Supporting Information

Molecular Dynamics Simulations, Reaction Pathway and Mechanism Dissection, and Kinetics Modeling of the Nitric Acid Oxidation of Dicyanamide (DCA^-) and Dicyanoborohydride ($DCBH^-$) Anions

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Details of Direct Dynamics Trajectory Simulations

Direct dynamics simulations of HNO_3 with DCA^- and $DCBH^-$ were carried out using the chemical dynamics program Venus of Hase *et al.*[1-2] coupled with the Gaussian 09 program package,[3] wherein Venus was used to set up the initial conditions for trajectories and the Hessian-based predictor-corrector algorithm,[4] implemented in Gaussian 09, was used to integrate the classical equations of motion. Direct dynamics calculates molecular energies, force constants and Hessians ″on the fly″ instead of using a pre-constructed analytical potential energy surface (PES). Molecules that are energized under specific conditions are able to explore multiple minima in the conformational landscape and on the reaction PES. Their motions are followed in time, from which the preferred reaction pathways and product structures are revealed. These unique features are vital for exploring hypergolic reactions wherein the heat of combustion of ionic liquids is large by virtue of their high heat of formation. Once combustion occurs upon heating, the resulting oxidation and decomposition processes of ionic liquids are vigorous. As a result, these processes are often controlled by dynamics (particularly at high temperatures) and may not follow the minimum-energy pathways.[5] Furthermore, reactions may be auto-catalytic[6] and non-statistical competition may arise among different product channels,[3-4] many of which could be beyond conventional chemical intuitions. Guided by direct dynamics simulations, it becomes feasible to identify new reaction mechanisms in hypergolic ionic liquids, explore energy dissipation pathways,[7-10] locate reaction activation barriers, and to determine rate-limiting steps.[7, 11-12]

Bimolecular collision trajectories started at the lowest-energy geometries of HNO_3 and DCA^- (or $DCBH^-$). Initial separation between the centers of mass of the randomly oriented reactants was set to 8.0 Å, at which point the inter-molecular interaction was negligible. Reactant vibrational modes and vibrational energies (E_{vib}, including zero-point energies in all vibrational modes) were sampled using quantum Boltzmann probability distributions at specific temperatures:[13]

$$P(n_i) = \exp(-\frac{n_i h\upsilon_i}{k_B T_{vib}}) \left[1 - \exp\left(-\frac{h\upsilon_i}{k_B T_{vib}}\right)\right] \quad \text{(S1)}$$

where ν_i and n_i are the vibrational frequency and quantum number of the i^{th} mode, respectively, and T_{vib} is the vibrational temperature. Quasi-classical initial molecular vibrations were simulated by giving individual atoms displacements (from equilibrium geometries) and momenta that are appropriate to initial rovibrational states, with random phases for different modes. Reactant rotational energies (E_{rot}) were sampled from classical Boltzmann distributions. Collision energy (E_{col}) was added as relative translational energy.

Trajectories were propagated at a step size of 0.25 $amu^{1/2}$Bohr, with the Hessian matrix updated every five steps. The trajectory propagation step size corresponds to ~ 0.4 fsec each step in trajectory time and is small enough for SCF convergence as well as to keep the total energy constant. The initial guess of

molecular orbital at each step was obtained from the previous step, and the total energy of the system was checked at each step to ensure that the energy was conserved to better than 10^{-4} Hartree. A quadratically convergent SCF procedure[14] was opted in to integrate the trajectory (i.e., SCF = XQC) in case the first-order SCF failed to converge within the allotted number of cycles. Because millions of gradient and Hessian evaluations were required for the trajectories, we had to make a compromise between accuracy and computational cost when choosing an appropriate theory for trajectory simulations. The B3LYP level of theory coupled with the 6-31+G(d) basis set was chosen in this work, as the dynamics simulations using this functional were able to reproduce the experimental results of imidazolium-DCA[15-16] and triazolium-DCA ILs.[5] Representative collision trajectories of DCA^- + HNO_3 and $DCBH^-$ + HNO_3 were recalculated at the ωB97XD/6-31+G(d) level of theory to test a range-separated functional for ionic liquid oxidation. It was found that ωB97XD/6-31+G(d) reproduced the reaction dynamics observed at B3LYP/6-31+G(d). Trajectories were terminated after a preset length of time (~ 3 psec) when product separation had exceeded 8.0 Å.

The simulations were carried out partly at the computing facility hosted by the AFRL Department of Defense Research Center′s High Performance Computing Modernization Program and partly on a computing cluster located at the CUNY Queens College. gOpenMol[17] was used for trajectory visualization. Trajectory reaction pathways were sorted and trajectory ensembles were analyzed by using in-house custom programs written for these purposes.

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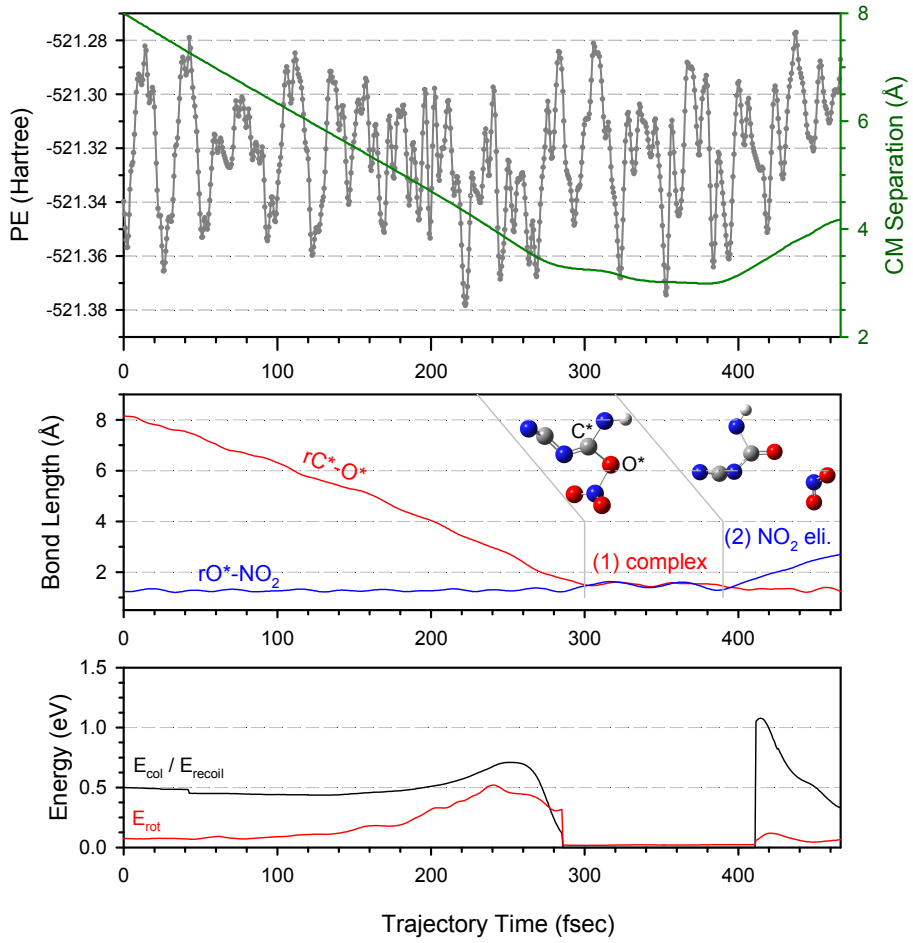

Figure S1. A representative trajectory of HNCNCN + NO_3^- → HNC(-ONO_2)NCN^-, followed by dissociation to [HNC(O)NCN]$^{\bullet-}$ + NO_2, simulated at 2000 K and E_{col} = 0.5 eV. Top frame shows the change of PE (left axis) and the reactants/products center-of-mass separation (right axis), middle frame shows the dissociation of rO-NO_2 and formation of rC-O, and bottom frame shows E_{col}, E_{recoil} and E_{rot}. Trajectory video is available in the Supporting Information.

Complex-forming Trajectories

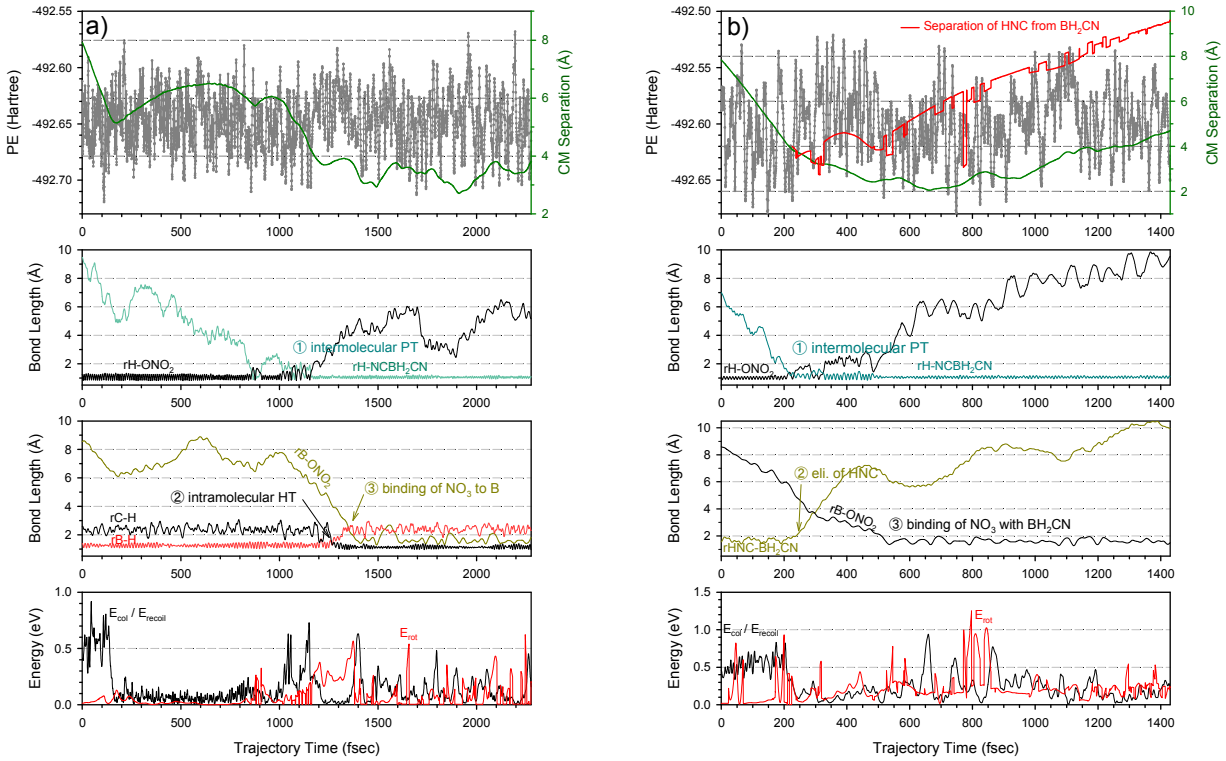

Figure S2. continued

H_2-elimination Trajectories

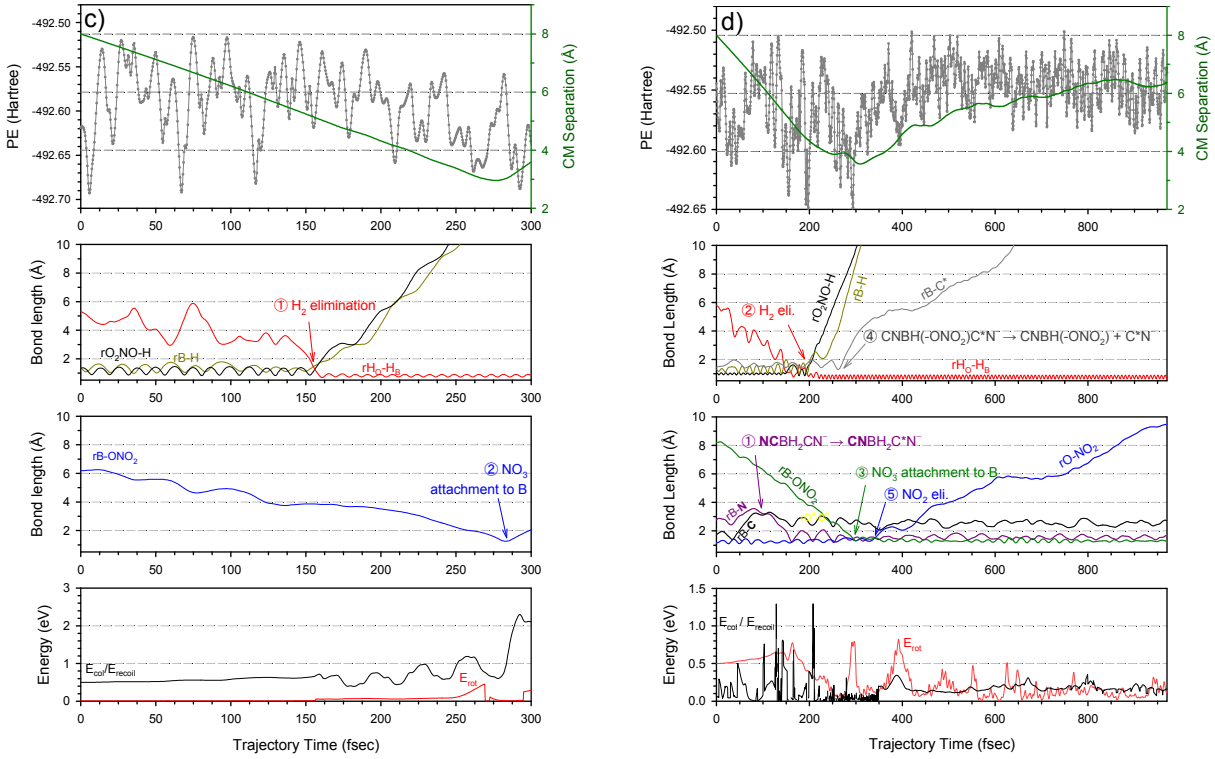

Figure S2. Trajectories of (a) $NCBH_2CN^- + HNO_3 \xrightarrow{①} NCBH_2CN^-\cdot HNO_3 \xrightarrow{②} O_3NH\cdot NCHBHCN^- \xrightarrow{③} HNCHBH(\text{-}ONO_2)CN^-$ simulated at 3000 K and E_{col} = 0.5 eV, (b) $NCBH_2CN^- + HNO_3 \xrightarrow{①} NCBH_2CN^-\cdot HNO_3 \xrightarrow{②} BH_2CN + O_2NO^-\cdot HNC \xrightarrow{③} BH_2(\text{-}ONO_2)CN^- + HNC$ simulated at 5000 K and 0.5 eV, (c) $DCBH^- + HNO_3 \xrightarrow{①} NCBHCN + NO_3^- + H_2 \xrightarrow{②} NCBH(\text{-}ONO_2)CN^- + H_2$ simulated at 5000 K and 0.5 eV and (d) $DCBH^- + HNO_3 \xrightarrow{①} O_3NH\cdot CNBH_2CN^- \xrightarrow{②} CNBHCN + NO_3^- + H_2 \xrightarrow{③} CNBH(\text{-}ONO_2)CN^- + H_2 \xrightarrow{④} CNBH(\text{-}ONO_2) + CN^- + H_2 \xrightarrow{⑤} [CNBHO]^\bullet + NO_2 + CN^- + H_2$ simulated at 5000 K and 0.5 eV. In each figure, top frame shows the change of PE (left axis) and the reactants/products center-of-mass separation (right axis), middle frames shows various bond lengths, and bottom frame shows E_{col}, E_{recoil} and E_{rot}. Trajectory videos are available in the Supporting Information.

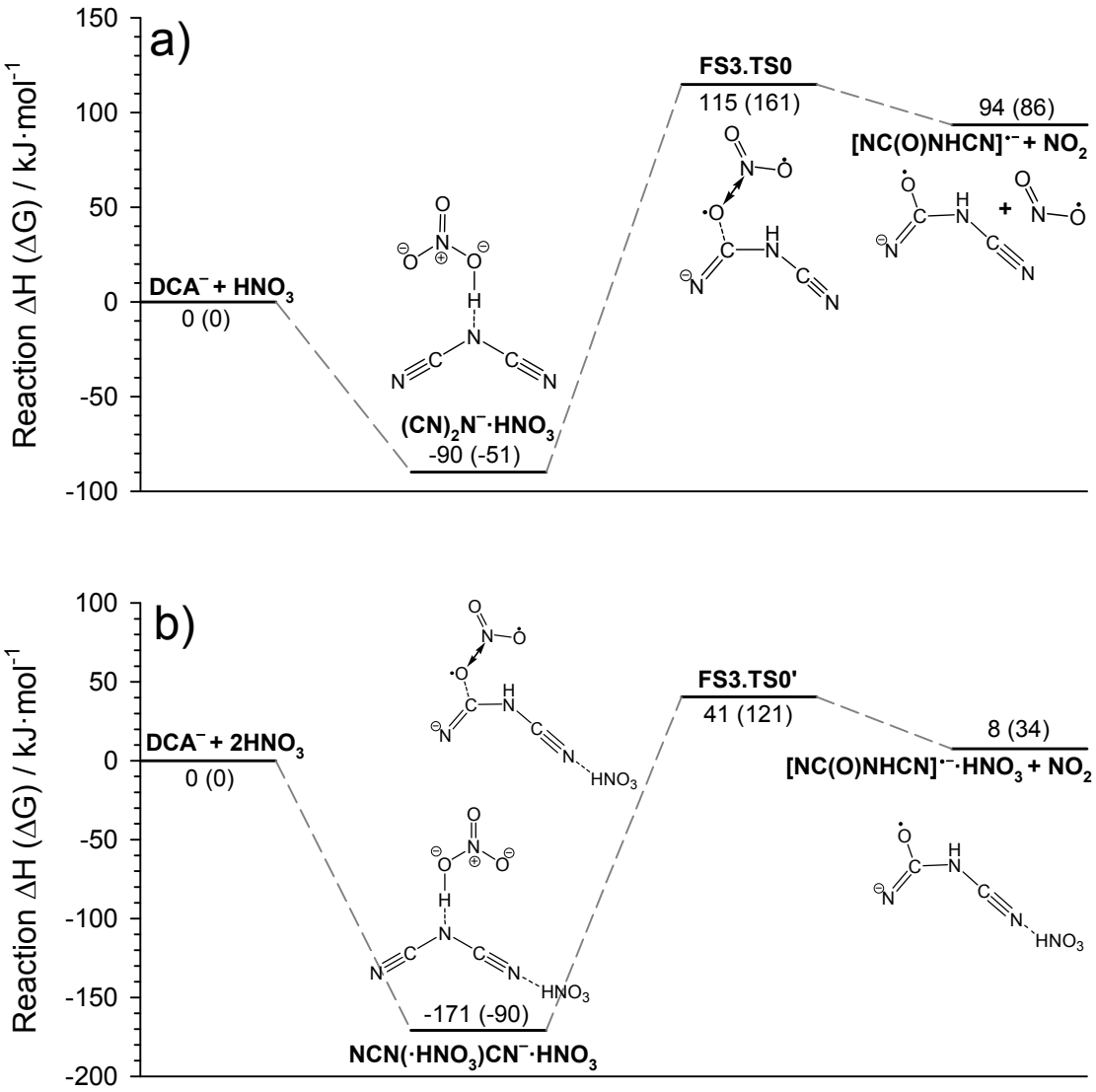

Figure S3. Reaction coordinates for the PT_{N3}-mediated reactions of DCA^- with (a) one and (b) two HNO_3. Structures and reaction ΔH (ΔG) at 298 K were calculated at the B3LYP/6-311++G(d,p) level of theory.

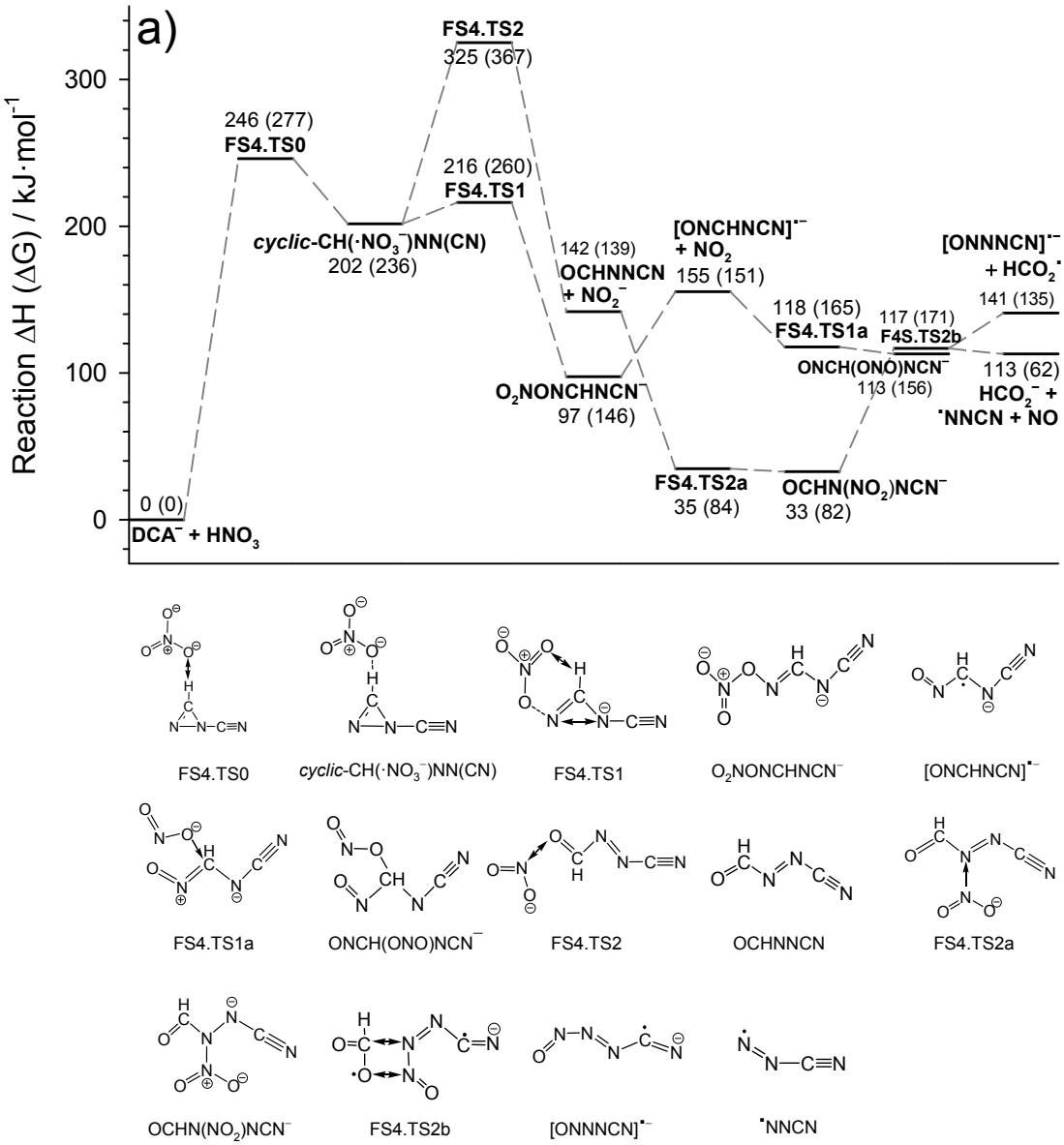

Figure S4. continued

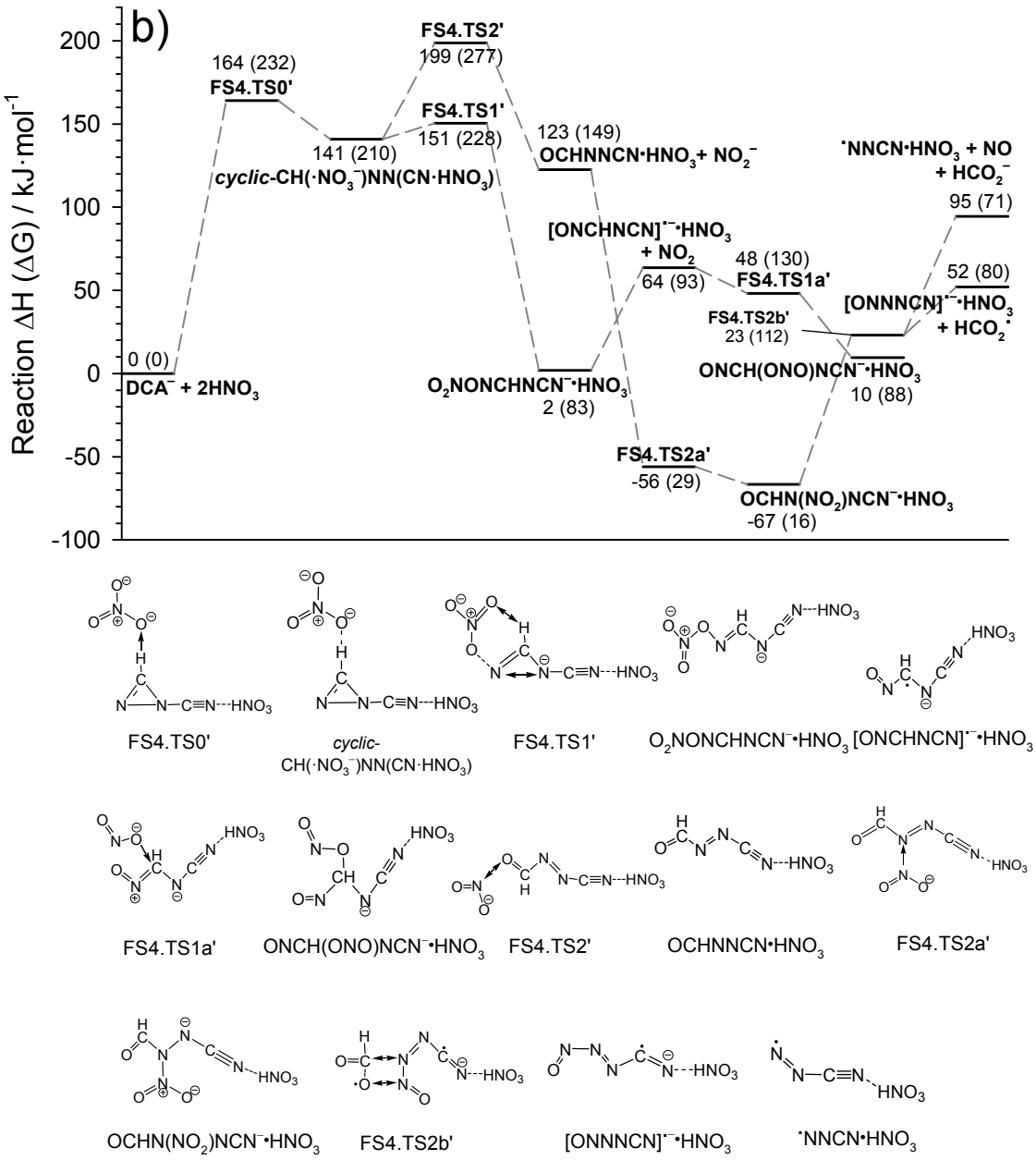

Figure S4. Reaction coordinates for the PT_{C2}-mediate reactions of DCA^- with (a) one and (b) two HNO_3. Structures and reaction ΔH (ΔG) at 298 K were calculated at the B3LYP/6-311++G(d,p) level of theory.

Cartesian coordinates for the structures in Figure 1a, calculated at B3LYP/ 6-311++G(d,p)

DCA^-
N1 2.234249 -0.389194 0.000000
C2 1.150169 0.058130 0.000000
N3 0.000000 0.678737 0.000000
C4 -1.150169 0.058130 0.000000
N5 -2.234249 -0.389194 0.000000

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$NCNCN^-\cdot HNO_3$
N1 2.790102 0.714845 -0.000677
C2 3.871641 -0.026735 0.000133
N3 4.895855 -0.588995 0.000788
C4 1.588447 0.255798 -0.000422
N5 0.456086 -0.042410 -0.000310
H6 -0.962275 -0.451917 -0.000277
N7 -2.904418 -0.000940 0.000133
O8 -1.922318 -0.920953 -0.000332
O9 -4.038798 -0.447362 0.000108
O10 -2.596587 1.180819 0.000532

F1.TS0
N1 1.593764 -0.412402 0.017551
O2 2.671764 -0.797824 -0.457557
O3 1.427298 -0.222279 1.234546
O4 0.605592 -0.210241 -0.792136
N5 -1.850736 0.563924 -0.187261
C6 -2.114261 -0.708008 0.017501
N7 -2.511153 -1.789447 0.177246
C8 -0.766150 1.196947 -0.105867
N9 -0.085950 2.212080 -0.012075
H10 -0.376233 2.890038 0.683144

$HNC(-ONO_2)NCN^-$
N1 1.444676 0.444004 -0.067776
O2 2.277668 1.106889 0.510810
O3 1.367196 0.216823 -1.252442
O4 0.475063 -0.078226 0.779407
H5 -0.621989 -2.868162 -0.278752
N6 -1.645378 -0.608054 -0.146458
C7 -1.988683 0.651639 -0.047710
N8 -2.410816 1.742823 -0.003374
C9 -0.439821 -1.067142 0.163447
N10 0.073459 -2.236303 0.115054

F1.TS1
N1 2.431909 0.333929 0.006244
O2 3.139557 0.012513 0.940086
O3 2.775435 0.963766 -0.973639
O4 0.021342 0.183615 0.406610
H5 -1.144830 -2.412674 -0.760350
C6 -2.936412 0.486563 0.120560
N7 -3.595013 1.429255 -0.243099
C8 -0.393890 -0.829495 -0.061634
N9 -0.272520 -1.914725 -0.647067
N10 -2.330666 -0.535442 0.515683

HNCO
C1 -0.044851 0.021878 -0.000210
N2 1.158127 -0.122263 0.000066
O3 -1.210324 0.013896 0.000085
H4 1.844813 0.613402 0.000122

$NCN^{\bullet-}$
C1 0.000000 0.000173 0.000047
N2 0.323272 -0.308407 1.141222
N3 -0.323272 0.308258 -1.141262

NO_2
N1 0.000000 0.000000 0.321839
O2 0.000000 1.099987 -0.140804
O3 0.000000 -1.099987 -0.140804

F1.TS2
N1 2.138190 -0.609979 -0.230264
O2 1.986580 0.141293 -1.150938
O3 2.701566 -0.484325 0.816519
O4 -0.055897 -0.823994 0.208245
H5 -0.003116 2.283023 0.132548
N6 -1.710933 0.780175 -0.013015
C7 -2.652509 -0.120819 -0.041749
N8 -3.597206 -0.816865 -0.099025
C9 -0.384831 0.397437 0.158078
N10 0.479830 1.417165 0.367857

$ONO\text{-}NHC(O)NCN^-$
N1 -2.815193 -0.185779 -0.163701
O2 -2.620546 -0.664188 0.881531
O3 -1.754821 0.672410 -0.668943
O4 0.290892 -1.104919 -0.632782
H5 -0.433102 1.803787 0.207640

N6 1.588351 0.654639 0.237715
C7 2.760042 0.066670 0.158730
N8 3.855372 -0.344623 0.132313
C9 0.477543 -0.005024 -0.131151
N10 -0.673760 0.818608 0.220592

F1.TS2a
N1 3.765046 -0.197669 -0.744788
O2 4.397876 -0.765953 0.036546
O3 0.860751 0.673246 0.937544
O4 -1.124013 2.120339 -0.326019
H5 -0.390860 -0.818573 0.704565
C6 -2.455471 -1.090108 -0.171768
N7 -2.607587 -2.238517 0.023856
C8 -1.291931 0.932145 -0.116236
N9 -0.236483 0.183701 0.556312
N10 -2.378354 0.187527 -0.429823

[ONHC(O)NCN]$^{\bullet-}$
N1 -0.716886 -0.678195 0.000084
C2 0.304555 0.203861 -0.000028
N3 1.530628 -0.576414 -0.000008
C4 -1.956383 -0.250111 0.000094
N5 -3.098145 0.008592 0.000114
O6 0.353952 1.423069 -0.000133
H7 1.399468 -1.589595 0.000080
O8 2.708838 -0.099418 -0.000092

NO
N1 0.000000 0.000000 -0.612285
O2 0.000000 0.000000 0.535749

F1.TS2b
N1 2.786511 -0.594308 -0.216360
O2 2.494267 0.536018 0.200072
O3 1.846438 -1.434265 -0.273315
O4 -0.543903 1.889414 -0.792698
H5 0.588913 -0.596757 0.348990
N6 -1.715202 0.370030 0.675942
C7 -2.368131 -0.594118 0.051159
N8 -3.035099 -1.427955 -0.419165
C9 -0.629535 1.022922 0.024894
N10 0.109884 0.237177 0.834186

OCNNCN^{-}
N1 -0.445049 -0.121483 -0.000436
C2 1.796718 0.053145 0.000042
C3 -1.635523 -0.063468 0.000013
O4 -2.832104 -0.152808 0.000193
N5 2.875589 -0.418186 0.000124
N6 0.667983 0.723155 0.000044

HONO
H1 1.720096 0.440472 0.000101
N2 -0.179880 0.486515 -0.000014
O3 -1.102769 -0.225490 0.000011
O4 1.045152 -0.255270 -0.000011

F1.TS3
N1 -1.744937 -0.246416 0.000094
O2 -2.202667 -0.412648 1.088267
O3 -2.204330 -0.410530 -1.087681
O4 -0.055857 -0.749483 -0.001447
H5 -0.559156 2.321948 0.002646
N6 1.645774 0.865773 0.000148
C7 2.562980 -0.073899 0.000002
N8 3.445236 -0.841552 -0.000033
C9 0.363250 0.508108 -0.000203
N10 -0.673986 1.315636 0.000568

O_2N-NHC(O)NCN^{-}
N1 2.957232 -0.992372 -0.186702
C2 2.123075 -0.163030 -0.142009
N3 1.303302 0.837348 -0.145212
C4 -0.023244 0.667887 0.202568
N5 -0.869537 1.644752 0.086015
N6 -1.900966 -1.122516 0.156268
O7 -2.435486 -0.484193 -0.596631
O8 -0.395332 -0.523822 0.664417
H9 -0.382659 2.464498 -0.278219

F1.TS3a
N1 1.602255 -0.199622 -0.629221
C2 0.737861 0.810248 -0.136958
N3 0.065939 -0.240709 0.379855
C4 2.698839 -0.517117 0.037858
N5 3.703098 -0.839515 0.533725
H6 -0.596707 -0.731883 -0.273491
O7 0.730924 2.003215 -0.157800
N8 -2.429239 -0.163802 0.217126
O9 -3.572681 0.146524 0.522818
O10 -2.235476 -1.014909 -0.695306

F1.TS3b
N1 1.603088 -0.683186 0.184382
C2 0.595830 0.200839 0.170693
N3 -0.613993 -0.565614 0.599544
C4 2.823827 -0.269046 -0.083067
N5 3.945361 -0.025310 -0.302751
H6 -0.492883 -1.528105 0.306535
O7 0.524242 1.385145 -0.084379

N8 -2.188189 -0.090444 -0.035002
O9 -2.539508 1.069765 0.053950
O10 -2.890850 -1.018757 -0.464008

[HNC(O)NCN]$^{\bullet-}$
O1 0.903651 1.352946 -0.047638
H2 1.852981 -1.536073 -0.271566
N3 -0.240305 -0.689716 -0.195165
C4 -1.444392 -0.215925 -0.014509
N5 -2.569439 0.087066 0.127250
C6 0.865179 0.119519 -0.035179
N7 2.008758 -0.641501 0.203744

Cartesian coordinates for the structures in Figure 1b, calculated at B3LYP/ 6-311++G(d,p)

DCA^-
N1 2.234249 -0.389194 0.000000
C2 1.150169 0.058130 0.000000
N3 0.000000 0.678737 0.000000
C4 -1.150169 0.058130 0.000000
N5 -2.234249 -0.389194 0.000000

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$O_3NH{\cdot}NCNCN^-{\cdot}HNO_3$
N1 5.627952 -0.194589 -0.000226
O2 6.710241 -0.746627 -0.000209
O3 4.558560 -1.028629 0.000047
O4 5.421825 1.006427 -0.000457
H5 3.681049 -0.471183 0.000005
N6 -0.000002 1.132555 -0.000024
C7 -1.149256 0.538752 -0.000029
N8 -2.235784 0.112483 -0.000036
C9 1.149255 0.538760 -0.000008
N10 2.235786 0.112499 0.000006
H11 -3.681050 -0.471191 -0.000033
O12 -4.558564 -1.028633 -0.000084
N13 -5.627951 -0.194587 0.000249
O14 -6.710244 -0.746619 0.000221
O15 -5.421818 1.006428 0.000541

F1.TS0′
N1 -2.892461 1.242130 0.047853
O2 -3.442266 2.278427 -0.341479
O3 -2.784083 0.948743 1.253945
O4 -2.406880 0.430637 -0.835083
H5 -3.828842 -2.361625 0.851291
N6 -1.102378 -1.778053 -0.168190
C7 -0.089129 -0.957153 -0.139761
N8 0.915206 -0.376684 -0.123430
C9 -2.338148 -1.532023 -0.071956
N10 -3.508485 -1.835154 0.050605
H11 2.351635 0.360036 -0.102344
O12 3.184936 0.957159 -0.115848
N13 4.286983 0.176490 0.049549
O14 5.341655 0.775461 0.047636
O15 4.125240 -1.023485 0.181660

$HNC(\text{-}ONO_2)NCN^-{\cdot}HNO_3$
N1 -1.133974 -1.622324 0.082041
C2 -2.359100 -1.164402 -0.203821
N3 -3.495206 -1.734487 -0.167648
C4 -0.062296 -0.905423 0.029859
N5 0.973370 -0.361538 0.023334
H6 -3.371527 -2.680524 0.188788
O7 -2.391783 0.192776 -0.741836
N8 -2.971402 1.161384 0.100062
O9 -3.113121 0.895583 1.267180
O10 -3.231513 2.187910 -0.478122
H11 2.323794 0.297086 -0.030585
O12 3.182396 0.912728 -0.087344
N13 4.302473 0.168128 0.013143
O14 5.347573 0.790512 -0.045474
O15 4.187610 -1.038978 0.151725

F1.TS1′
N1 4.237359 -1.091706 -0.013299
O2 4.686800 -1.459588 -1.070901
O3 4.584666 -1.397834 1.100738
O4 2.129644 -0.003145 -0.148070
H5 2.447534 3.060434 -0.121276
C6 -0.612360 1.032059 0.260099
N7 -1.532710 0.436776 0.770006
C8 2.307726 1.173346 -0.133493
N9 2.984006 2.203742 -0.108555
N10 0.292790 1.712800 -0.246470
H11 -2.756543 -0.414065 0.382379
O12 -3.509897 -1.118015 0.176893
N13 -4.664717 -0.473177 -0.106183
O14 -4.667202 0.746471 -0.076077
O15 -5.609046 -1.192619 -0.368736

$[NCNH]^{\bullet}{\cdot}NO_3^-$
C1 -2.525754 -0.012752 -0.005824
N2 -1.648606 -0.340483 -0.853526
N3 -3.433009 0.287725 0.712295
H4 -0.649340 -0.471409 -0.490146
O5 0.833428 -0.929295 0.048408
N6 1.671615 0.041979 0.049891
O7 1.280601 1.177247 -0.299032
O8 2.845204 -0.170030 0.396182

HNCO
C1 -0.044851 0.021878 -0.000210
N2 1.158127 -0.122263 0.000066
O3 -1.210324 0.013896 0.000085

H4 1.844813 0.613402 0.000122

NO_2
N1 0.000000 0.000000 0.321839
O2 0.000000 1.099987 -0.140804
O3 0.000000 -1.099987 -0.140804

F1.TS2′
N1 -4.157799 -0.943653 0.346852
O2 -4.234034 -0.019249 1.098882
O3 -4.617687 -1.176561 -0.725605
O4 -2.057039 -0.672134 0.009597
H5 -2.918255 2.316774 -0.239872
N6 -0.824944 1.276752 -0.174231
C7 0.295446 0.633824 -0.175967
N8 1.377504 0.185492 -0.175624
C9 -2.025567 0.589637 -0.149679
N10 -3.129407 1.332165 -0.387168
H11 2.765134 -0.409753 -0.141504
O12 3.653089 -0.980507 -0.156469
N13 4.722129 -0.190739 0.076285
O14 4.535048 1.000369 0.263949
O15 5.798305 -0.760405 0.076203

ONO-NHC(O)NCN^{-}·HNO_3
N1 -0.796801 -0.806176 -0.089670
C2 -1.887232 -0.060064 0.218114
N3 -3.063112 -0.830410 -0.089715
C4 0.389513 -0.298583 -0.022740
N5 1.506659 0.045182 0.002167
O6 -1.993263 1.078581 0.638982
H7 -2.910721 -1.830917 -0.039771
H8 2.917343 0.466204 0.029509
O9 3.879737 0.933040 0.068967
N10 4.859588 0.021745 -0.064793
O11 5.994964 0.464936 -0.029888
O12 4.550696 -1.151468 -0.207882
O13 -4.178951 -0.523248 0.686477
N14 -5.146005 0.361465 -0.014886
O15 -4.821008 0.694902 -1.077121

F1.TS2a′
No converged structure was located. The energy was determined from a relaxed PES scan.

[ONHC(O)NCN]$^{\bullet-}$·HNO_3
N1 -1.729723 -0.640150 -0.000102
C2 -2.794218 0.204808 0.000006
N3 -3.985261 -0.614704 -0.000010
C4 -0.521838 -0.180363 -0.000109
N5 0.608897 0.116473 -0.000127
O6 -2.872896 1.417303 0.000106
H7 -3.827142 -1.624120 -0.000108
H8 2.058980 0.472522 -0.000100
O9 3.035263 0.890628 -0.000097
N10 3.966492 -0.083115 0.000037
O11 5.122541 0.301379 0.000064
O12 3.593630 -1.245698 0.000118
O13 -5.173328 -0.169188 0.000088

NO
N1 0.000000 0.000000 -0.612285
O2 0.000000 0.000000 0.535749

F1.TS2b′
N1 4.311313 1.675754 0.143837
O2 4.655559 0.495374 0.042121
O3 3.091168 1.925634 -0.095814
O4 2.437591 -1.892201 1.187363
H5 2.529259 0.586526 -0.495049
N6 0.949378 -1.422082 -0.671565
C7 -0.130640 -0.750950 -0.354666
N8 -1.152122 -0.229181 -0.151146
C9 2.113791 -1.345510 0.179145
N10 2.512746 -0.489844 -0.769431
H11 -2.623872 0.444707 0.142381
O12 -3.439475 1.003365 0.386639
N13 -4.561652 0.297784 0.059832
O14 -4.417603 -0.805608 -0.432309
O15 -5.604981 0.863499 0.302639

OCNNCNH·NO_3^{-}
N1 -2.685655 0.036422 0.255448
C2 -0.731492 1.058809 -0.172040
C3 -3.772231 -0.464440 0.115862
O4 -4.830751 -0.987181 0.152163
N5 0.292427 1.572890 0.157026
N6 -1.837992 0.680568 -0.647294
H7 1.310950 1.158677 0.177952
O8 2.760342 0.800047 0.255784
N9 3.037575 -0.439262 0.014161
O10 2.107770 -1.222328 -0.254468
O11 4.221002 -0.800441 0.059486

HONO
H1 1.720096 0.440472 0.000101
N2 -0.179880 0.486515 -0.000014
O3 -1.102769 -0.225490 0.000011
O4 1.045152 -0.255270 -0.000011

F1.TS3'
N1 3.183854 -1.093952 0.112208
O2 3.591446 -2.015063 -0.550867
O3 3.373673 -0.859256 1.276631
O4 2.306755 -0.244519 -0.606445
H5 3.272740 2.682202 0.175150
N6 1.037179 1.629840 -0.034217
C7 -0.032530 0.908275 -0.058624
N8 -1.070566 0.368894 -0.057508
C9 2.277051 1.146213 -0.186203
N10 3.411475 1.715978 -0.112182
H11 -2.406828 -0.309408 -0.081717
O12 -3.257772 -0.939477 -0.126857
N13 -4.386039 -0.221206 0.042941
O14 -4.288293 0.982922 0.217124
O15 -5.421352 -0.861683 0.005018

O_2N-NHC(O)$NCN^{-}\cdot HNO_3$
N1 0.838378 -0.598299 -0.200657
C2 1.875579 0.264968 -0.106847
N3 3.078975 -0.551463 -0.269563
C4 -0.378858 -0.158891 -0.122664
N5 -1.512151 0.115964 -0.067251
O6 1.926242 1.461841 0.064567
H7 2.954316 -1.544135 -0.121664
N8 4.360207 -0.171728 0.054399
O9 5.118110 -1.104214 0.352008
O10 4.675405 0.999782 -0.017444
H11 -2.989367 0.463077 0.003506
O12 -3.958253 0.871182 0.055143
N13 -4.879822 -0.116217 0.053902
O14 -6.037389 0.255148 0.111035
O15 -4.492163 -1.271639 -0.002882

F1.TS3a'
N1 0.852552 0.550634 0.767835
C2 1.839189 1.124417 -0.101157
N3 2.193052 -0.162745 -0.242703
C4 -0.341475 0.261540 0.305904
N5 -1.433645 0.003861 -0.000664
H6 2.851533 -0.571841 0.499512
O7 2.083925 2.225619 -0.480343
N8 4.642931 -0.645395 -0.226435
O9 5.797030 -0.760780 -0.600684
O10 4.314269 -1.063362 0.925181
H11 -3.002106 -0.343986 -0.433718
O12 -3.878829 -0.639259 -0.850279
N13 -4.897159 -0.261584 -0.018492
O14 -4.605178 0.328419 1.004018
O15 -6.003694 -0.564800 -0.404276

O_2N-NHC(O)NCNH$\cdot NO_3^{-}$
N1 0.838378 -0.598299 -0.200657
C2 1.875579 0.264968 -0.106847
N3 3.078975 -0.551463 -0.269563
C4 -0.378858 -0.158891 -0.122664
N5 -1.512151 0.115964 -0.067251
O6 1.926242 1.461841 0.064567
H7 2.954316 -1.544135 -0.121664
N8 4.360207 -0.171728 0.054399
O9 5.118110 -1.104214 0.352008
O10 4.675405 0.999782 -0.017444
H11 -2.989367 0.463077 0.003506
O12 -3.958253 0.871182 0.055143
N13 -4.879822 -0.116217 0.053902
O14 -6.037389 0.255148 0.111035
O15 -4.492163 -1.271639 -0.002882

F1.TS3b′
N1 0.549005 -0.470053 0.380657
C2 1.619998 0.387235 0.107372
N3 2.426035 -0.321604 -0.744781
C4 -0.671675 -0.107993 0.173034
N5 -1.809392 0.119160 0.011571
O6 1.752790 1.542736 0.450295
H7 2.570747 -1.265517 -0.383324
N8 5.457050 -0.203301 -0.090369
O9 5.929611 -1.322465 -0.037713
O10 6.047572 0.844330 0.030109
H11 -3.384778 0.423363 -0.197949
O12 -4.323047 0.775750 -0.407565
N13 -5.239848 -0.157749 -0.027275
O14 -6.394656 0.150484 -0.231942
O15 -4.831752 -1.190644 0.470593

$[HNC(O)NCN]^{\bullet-}\cdot HNO_3$
O1 -3.413523 -1.317191 -0.261712
H2 -4.524335 1.465111 -0.229756
N3 -2.279886 0.714739 -0.010379
C4 -1.076418 0.247230 0.025560
N5 0.053536 -0.054545 0.064821
C6 -3.369567 -0.109008 -0.034347
N7 -4.560906 0.570954 0.272878
H8 1.483656 -0.438718 0.107484
O9 2.453505 -0.878137 0.172506
N10 3.410950 0.049940 -0.010022
O11 3.072418 1.204966 -0.216587
O12 4.556441 -0.362554 0.050033

F1.TS3c'

N1 -0.067548 1.286079 -0.720253
C2 -0.952519 0.759483 0.184648
N3 -2.025750 0.178973 -0.592835
C4 1.174751 1.402422 -0.510121
N5 2.261777 1.966978 -0.526434
O6 -0.947159 0.786731 1.386007
H7 -1.766198 -0.208177 -1.491336
N8 -3.113646 -0.489884 -0.063208
O9 -3.595413 -1.357604 -0.794636
O10 -3.542224 -0.149465 1.020757
H11 2.222324 2.972278 -0.387516
O12 1.632589 -0.565331 -0.424410
N13 2.724113 -0.990417 0.154441
O14 3.141440 -0.407395 1.158033
O15 3.280498 -1.981640 -0.337037

O_2N-NHC(O)NC(-ONO_2)NH^-

N1 -0.092287 1.262522 -0.109402
C2 0.628483 0.132631 -0.188196
N3 2.038839 0.583800 -0.241881
C4 -1.430999 1.289485 -0.193957
N5 -2.240142 2.252403 0.017967
O6 0.354388 -1.049301 -0.203588
H7 2.183585 1.528310 0.089067
N8 3.139394 -0.187892 0.031408
O9 4.107888 0.425691 0.507102
O10 3.128887 -1.372373 -0.247272
H11 -1.692427 3.052361 0.334256
O12 -2.098221 0.118500 -0.751671
N13 -2.477041 -0.849410 0.183821
O14 -2.999600 -1.813519 -0.320268
O15 -2.275517 -0.626914 1.352723

F1.TS3d'

N1 -0.099266 0.784113 -0.001240
C2 -1.030853 -0.190380 -0.004892
N3 -2.302926 0.512619 0.300171
C4 1.206598 0.468515 -0.094566
N5 2.154710 1.389403 -0.217527
O6 -1.011917 -1.383680 -0.200069
H7 -2.269535 1.511881 0.148547
N8 -3.563066 0.036286 0.047803
O9 -4.418588 0.905014 -0.185508
O10 -3.780510 -1.159526 0.115529
H11 1.931379 2.330821 0.092527
O12 1.698428 -0.743218 -0.069816
N13 3.414162 -0.148580 0.054025
O14 3.777303 -0.210734 1.193816
O15 3.992582 -0.348905 -0.969821

DNB^-

N1 -0.000001 -0.212264 0.000004
C2 1.166734 0.467962 -0.046609
O3 1.473973 1.630260 0.056184
N4 2.200703 -0.579519 -0.256337
N5 3.544652 -0.431116 -0.019846
O6 4.133793 -1.460384 0.344319
O7 4.074403 0.645315 -0.223365
C8 -1.166736 0.467962 0.046610
O9 -1.473976 1.630259 -0.056197
N10 -2.200703 -0.579519 0.256349
N11 -3.544651 -0.431117 0.019848
O12 -4.133786 -1.460383 -0.344334
O13 -4.074407 0.645310 0.223376
H14 -1.904221 -1.511910 0.000566
H15 1.904223 -1.511912 -0.000558

Cartesian coordinates for the structures in Figure S3a, calculated at B3LYP/ 6-311++G(d,p)

DCA^-
N1 2.234249 -0.389194 0.000000
C2 1.150169 0.058130 0.000000
N3 0.000000 0.678737 0.000000
C4 -1.150169 0.058130 0.000000
N5 -2.234249 -0.389194 0.000000

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$(CN)_2N^- \cdot HNO_3$
N1 -2.397071 2.201894 -0.080599
C2 -1.908997 1.147299 0.012990
N3 -1.262465 -0.000002 0.142601
C4 -1.909170 -1.147203 0.012976
N5 -2.397397 -2.201725 -0.080639
N6 2.140008 -0.000002 -0.069247
H7 0.225768 -0.000097 0.478480
O8 1.199649 -0.000148 0.903778
O9 1.771834 -0.000051 -1.231305
O10 3.291232 -0.000004 0.325140

FS3.TS0
N1 -1.102177 2.093366 -0.000235
C2 -0.571862 1.001325 0.000100
N3 -1.067105 -0.345594 0.000716
C4 -2.355337 -0.656691 0.000072
N5 -3.474394 -0.970556 -0.000377
N6 1.950075 -0.343273 -0.000029
H7 -0.372717 -1.093707 0.000337
O8 1.504665 -1.481546 -0.000201
O9 0.860573 1.008743 0.000025
O10 3.108652 -0.028658 -0.000060

$[NC(O)NHCN]^{\bullet-}$
N1 -0.903271 1.428120 0.035228
C2 -1.040372 0.144400 0.010209
N3 0.252048 -0.645581 0.163258
C4 1.488071 -0.198119 0.008951
N5 2.585566 0.178869 -0.096464
H6 0.089451 -1.628228 -0.012478
O7 -2.039506 -0.597415 -0.102079

NO_2
N1 0.000000 0.000000 0.321839
O2 0.000000 1.099987 -0.140804
O3 0.000000 -1.099987 -0.140804

Cartesian coordinates for the structures in Figure S3b, calculated at B3LYP/ 6-311++G(d,p)

DCA^-
N1 2.234249 -0.389194 0.000000
C2 1.150169 0.058130 0.000000
N3 0.000000 0.678737 0.000000
C4 -1.150169 0.058130 0.000000
N5 -2.234249 -0.389194 0.000000

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$NCN(\cdot HNO_3)CN^- \cdot HNO_3$
N1 -2.078024 3.506433 -0.046507
C2 -1.621217 2.436180 -0.070852
N3 -1.203740 1.179251 -0.128128
C4 0.043462 0.874977 0.106859
N5 1.131085 0.504041 0.297824
N6 -3.594101 -1.339653 0.068530
H7 -2.287217 0.001855 -0.498375
O8 -2.925472 -0.681248 -0.924845
O9 -3.335802 -1.047434 1.220409
O10 -4.391626 -2.165250 -0.319365
H11 2.626197 0.053580 0.564430
O12 3.555119 -0.209563 0.930894
N13 4.378213 -0.521908 -0.104685
O14 5.504770 -0.840989 0.216355
O15 3.929701 -0.457955 -1.234863

FS3.TS0'
N1 1.913957 2.474596 -0.000105
C2 2.076496 1.271724 0.000084
N3 1.135799 0.161598 0.000709
C4 -0.165713 0.327627 0.000775
N5 -1.319714 0.447795 0.000875
N6 3.949753 -0.864176 -0.000269
H7 1.524802 -0.785107 0.000775
O8 3.132913 -1.771922 0.000312
O9 3.405409 0.796266 -0.000351
O10 5.142405 -0.965582 -0.000802
H11 -2.942913 0.560306 0.000199
O12 -3.938625 0.792073 -0.000320
N13 -4.653910 -0.367997 -0.000247
O14 -4.038200 -1.418358 0.000416
O15 -5.857375 -0.224230 -0.000864

$[NC(O)NHCN]^{\bullet-} \cdot HNO_3$
N1 -3.388739 1.435870 0.023768
C2 -3.598083 0.167475 -0.028781
N3 -2.292969 -0.676904 0.170867
C4 -1.056753 -0.259601 0.107722
N5 0.042975 0.120345 0.076598
H6 -2.470623 -1.662302 0.027073
O7 -4.589621 -0.556498 -0.190141
H8 1.561517 0.529408 0.023428
O9 2.510818 0.941840 -0.008784
N10 3.429689 -0.055614 -0.029982
O11 3.029940 -1.207166 -0.011299
O12 4.586540 0.311795 -0.066389

NO_2
N1 0.000000 0.000000 0.321839
O2 0.000000 1.099987 -0.140804
O3 0.000000 -1.099987 -0.140804

Cartesian coordinates for the structures in Figure S4a, calculated at B3LYP /6-311++G(d,p)

DCA^-
N1 2.234249 -0.389194 0.000000
C2 1.150169 0.058130 0.000000
N3 0.000000 0.678737 0.000000
C4 -1.150169 0.058130 0.000000
N5 -2.234249 -0.389194 0.000000

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

FS4.TS0
N1 -3.851874 -0.967286 -0.690369
C2 -3.012294 -0.464525 -0.034871
N3 -2.144523 -0.012542 0.825774
C4 -0.886321 0.643930 0.205991
N5 -1.328637 1.723957 -0.067207
H6 0.429061 -0.093347 0.189722
O7 1.303594 -0.797099 0.260821
N8 2.442343 -0.166631 -0.070396
O9 2.383696 1.011769 -0.394703
O10 3.455393 -0.842866 -0.016251

***cyclic*-CH(·NO_3^-)NN(CN)**
N1 -3.852144 -1.109156 -0.573727
C2 -3.058888 -0.454461 -0.033232
N3 -2.240532 0.286063 0.732026
C4 -0.913652 0.531336 0.194634
N5 -1.538150 1.541847 -0.143809
H6 0.076196 -0.004690 0.201739
O7 1.523241 -0.918894 0.296837
N8 2.507101 -0.170733 -0.045090
O9 2.271183 1.013006 -0.384102
O10 3.658715 -0.630700 -0.032230

FS4.TS1
N1 4.005186 -0.456280 0.836835
C2 3.119445 -0.192816 0.124324
N3 2.219918 0.100430 -0.800926
C4 0.851733 -0.033098 -0.451786
N5 0.784179 1.163047 -0.148559
H6 0.121868 -0.848507 -0.483616
O7 -1.810177 -1.195261 -0.247326
N8 -2.364886 -0.113855 0.105115
O9 -1.658365 0.928760 0.263940
O10 -3.588923 -0.064674 0.296029

$O_2NONCHNCN^-$
N1 -4.119779 0.194888 -0.777959
C2 -3.137904 0.113164 -0.143789
N3 -2.102257 0.048035 0.657817
C4 -0.917217 -0.264245 0.145879
N5 0.157915 -0.357762 0.904761
H6 -0.807570 -0.468579 -0.927168
O7 2.034589 1.290212 0.180357
N8 2.240724 0.155031 -0.160238
O9 1.220650 -0.833683 0.061792
O10 3.232520 -0.319813 -0.674155

$[ONCHNCN]^{\bullet-}$
N1 -2.917898 0.373411 0.000017
C2 -1.822721 -0.045576 -0.000006
N3 -0.649595 -0.626970 -0.000003
C4 0.454176 0.114347 -0.000048
N5 1.672525 -0.456218 0.000022
H6 0.418769 1.212755 0.000019
O7 2.632159 0.417882 0.000006

NO_2
N1 0.000000 0.000000 0.321839
O2 0.000000 1.099987 -0.140804
O3 0.000000 -1.099987 -0.140804

FS4.TS1a
N1 -3.531286 -1.151706 0.366865
C2 -2.643929 -0.489935 0.003802
N3 -1.720596 0.302687 -0.515361
C4 -0.653672 0.586083 0.154103
N5 0.233056 1.561907 -0.413024
H6 -0.449750 0.291006 1.184336
O7 1.029075 -0.844007 -0.427889
N8 2.121446 -0.553987 0.133789
O9 1.017630 1.995960 0.416500
O10 3.017922 -1.399479 0.119183

$ONCH(ONO)NCN^-$
N1 -3.041049 -1.453982 0.468939
C2 -2.191917 -0.821362 -0.038526
N3 -1.306643 -0.118158 -0.693602
C4 -0.195174 0.316107 -0.024714
N5 -0.011755 1.758265 -0.416801
H6 -0.146621 0.216159 1.065466
O7 1.080080 -0.338610 -0.549618

N8 1.872262 -0.786530 0.471367
O9 0.028177 2.502873 0.539941
O10 2.876676 -1.286988 0.072759

FS4.TS2
N1 3.636642 -1.138912 0.375429
C2 2.746424 -0.504246 -0.036778
N3 1.745234 0.159335 -0.608733
C4 0.317655 0.507547 0.248603
N5 1.359835 1.381687 0.114054
H6 0.196457 -0.235004 1.047601
O7 -2.793151 -0.876789 -0.883351
N8 -2.285806 -0.280215 0.033920
O9 -0.678652 0.889599 -0.469365
O10 -2.749731 -0.092570 1.137561

OCHNNCN
N1 -2.950237 -0.223932 -0.000351
C2 -1.817618 0.016113 0.000302
N3 -0.547645 0.489592 -0.000459
C4 1.659310 0.308194 0.000269
N5 0.359733 -0.373980 0.000832
H6 1.581334 1.410555 0.000871
O7 2.666944 -0.324770 -0.000556

NO_2^-
N1 0.000000 0.458837 0.000000
O2 1.071093 -0.200866 0.000000
O3 -1.071093 -0.200617 0.000000

FS4.TS2a
N1 3.238794 -0.050106 -0.488775
C2 2.197790 0.297815 -0.087714
N3 1.098631 0.745155 0.507303
C4 -1.019253 1.520514 0.119063
N5 -0.007235 0.614220 -0.218275
H6 -0.572349 2.458988 0.502390
O7 -2.209527 1.394047 -0.060725
N8 -0.752126 -1.102952 0.034292
O9 -1.604015 -1.499286 -0.726736
O10 -0.129624 -1.746409 0.845924

$OCHN(NO_2)NCN^-$
N1 -3.126186 -0.263736 -0.630598
C2 -2.113219 -0.430855 -0.064803
N3 -1.055702 -0.674620 0.690591
C4 1.118647 -1.365068 0.041791
N5 0.137223 -0.373772 0.052330
H6 0.599167 -2.328023 0.169876
O7 2.318898 -1.256537 -0.068121
N8 0.564718 1.041616 0.018858
O9 1.553532 1.301764 -0.645079
O10 -0.156443 1.829416 0.594441

FS4.TS2b
N1 3.347416 0.198345 -0.143049
C2 2.276167 -0.250438 0.009499
N3 1.149156 -0.886138 0.261009
C4 -0.757756 1.301482 0.364746
N5 0.039364 -0.178946 -0.033108
H6 -0.784430 1.244002 1.460217
O7 -0.644468 2.283746 -0.306715
N8 -1.104130 -0.787892 -0.105039
O9 -2.024114 0.202005 -0.002920
O10 -1.375003 -1.981732 -0.135913

$[ONNNCN]^{\bullet-}$
N1 -2.812505 -0.054173 0.061563
C2 -1.644733 -0.114137 -0.013729
N3 -0.351472 -0.342523 -0.128439
N4 0.409124 0.739431 0.045294
N5 1.722159 0.512720 -0.045409
O6 2.137156 -0.662921 0.068914

$HCO_2^\bullet$
C1 0.000029 0.433109 -0.000001
H2 -0.000025 1.530982 0.000002
O3 1.044221 -0.258107 0.000000
O4 -1.044240 -0.258097 0.000000

$[NNCN]^\bullet$
N1 1.780247 -0.122019 0.000002
C2 0.632393 0.016869 -0.000003
N3 -0.682186 0.401379 0.000001
N4 -1.640111 -0.293819 0.000000

NO
N1 0.000000 0.000000 -0.612285
O2 0.000000 0.000000 0.535749

HCO_2^-
C1 -0.000190 0.314526 0.000001
H2 0.002101 1.453693 -0.000001
O3 1.137559 -0.208962 0.000000
O4 -1.137679 -0.208644 0.000000

Cartesian coordinates for the structures in Figure S4b, calculated at B3LYP/ 6-311++G(d,p)

DCA^-
N1 2.234249 -0.389194 0.000000
C2 1.150169 0.058130 0.000000
N3 0.000000 0.678737 0.000000
C4 -1.150169 0.058130 0.000000
N5 -2.234249 -0.389194 0.000000

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

FS4.TS0'
N1 1.674222 0.318140 -0.031931
C2 0.638934 0.760172 -0.364534
N3 -0.441920 1.231013 -0.900199
C4 -1.719511 1.119149 -0.029606
N5 -1.449299 2.079795 0.640740
H6 -2.930576 -0.008100 -0.299057
O7 -3.571668 -0.780790 -0.614109
N8 -4.740125 -0.695147 0.077330
O9 -4.853499 0.193654 0.903363
O10 -5.567548 -1.534603 -0.209112
H11 3.078991 -0.162070 0.433365
O12 3.934057 -0.517673 0.907895
N13 4.983291 -0.467899 0.051588
O14 4.787846 -0.049146 -1.076105
O15 6.039794 -0.857327 0.509047

***cyclic*-CH(·NO_3^-)NN(CN·HNO_3)**
N1 1.605415 0.278384 0.002829
C2 0.591983 0.795701 -0.222654
N3 -0.488631 1.465241 -0.617482
C4 -1.766870 1.046589 -0.038318
N5 -1.410526 1.971885 0.695194
H6 -2.567834 0.271506 -0.296572
O7 -3.652192 -0.847595 -0.738860
N8 -4.704811 -0.710083 -0.007875
O9 -4.708598 0.186101 0.865795
O10 -5.670233 -1.459677 -0.189816
H11 3.110336 -0.415362 0.337456
O12 3.914475 -0.931330 0.664347
N13 5.018957 -0.452017 0.008806
O14 4.853151 0.441368 -0.798832
O15 6.058898 -0.986834 0.316697

FS4.TS1'
N1 -1.649569 0.296613 -0.127635
C2 -0.609754 0.778476 0.074925
N3 0.483576 1.442679 0.378818
C4 1.740550 0.775348 0.234429
N5 1.810443 1.230085 -0.909252
H6 2.397486 0.167794 0.881895
O7 3.999218 -0.704277 1.137245
N8 4.667157 -0.569502 0.062356
O9 4.154154 0.061782 -0.907026
O10 5.802151 -1.049921 -0.030899
H11 -3.161837 -0.345965 -0.397198
O12 -3.999659 -0.836386 -0.690919
N13 -5.049837 -0.370376 0.051945
O14 -4.820689 0.490175 0.880294
O15 -6.116777 -0.880282 -0.205502

$O_2NONCHNCN^-\cdot HNO_3$
N1 1.843294 0.968674 0.029628
C2 0.694843 1.163956 -0.089612
N3 -0.545328 1.499329 -0.214490
C4 -1.486738 0.556397 -0.346767
N5 -2.746157 0.883659 -0.478830
H6 -1.214555 -0.504970 -0.361842
O7 -4.500756 0.097588 1.237473
N8 -4.479406 -0.581009 0.245930
O9 -3.461538 -0.338587 -0.734232
O10 -5.221059 -1.478304 -0.087774
H11 3.315774 0.677243 0.172679
O12 4.361140 0.652809 0.321112
N13 4.842649 -0.581831 0.063717
O14 4.057724 -1.450895 -0.279081
O15 6.045088 -0.709628 0.203221

$[ONCHNCN]^{\bullet-}\cdot HNO_3$
N1 0.276408 0.715818 0.000260
C2 -0.894287 0.755344 0.000471
N3 -2.174010 0.930407 0.000850
C4 -3.016940 -0.104162 -0.000151
N5 -4.344181 0.100969 0.000245
H6 -2.664582 -1.143260 -0.001317
O7 -5.013474 -1.005544 -0.000861
H8 1.808549 0.687917 -0.000297
O9 2.841265 0.865698 -0.000862
N10 3.514693 -0.307813 -0.000048
O11 2.871934 -1.343778 0.001177
O12 4.726904 -0.207303 -0.000637

NO_2
N1 0.000000 0.000000 0.321839
O2 0.000000 1.099987 -0.140804
O3 0.000000 -1.099987 -0.140804

FS4.TS1a'
N1 1.401916 0.003679 -0.554879
C2 0.315501 -0.403766 -0.645498
N3 -0.862193 -0.926910 -0.869719
C4 -1.807217 -0.860158 0.018897
N5 -3.020021 -1.555926 -0.263776
H6 -1.691420 -0.472933 1.031772
O7 -3.027688 0.991377 -0.368795
N8 -4.081597 0.993778 0.316109
O9 -3.756641 -1.586595 0.714937
O10 -4.739139 2.026244 0.397678
H11 2.940876 0.513292 -0.383726
O12 3.850647 0.977509 -0.371039
N13 4.747828 0.160916 0.252920
O14 4.349349 -0.910600 0.670358
O15 5.873385 0.603869 0.325232

$ONCH(ONO)NCN^{-}\cdot HNO_3$
N1 1.245046 -0.613019 -0.705542
C2 0.077686 -0.685163 -0.805142
N3 -1.182835 -0.811043 -1.016881
C4 -2.087024 -0.426569 -0.041043
N5 -2.961583 -1.642681 0.218580
H6 -1.697965 -0.054711 0.913420
O7 -3.032647 0.576079 -0.559562
N8 -3.204068 1.624367 0.343852
O9 -2.894476 -2.026624 1.361407
O10 -3.985154 2.416100 -0.053386
H11 2.700978 -0.473954 -0.582397
O12 3.771523 -0.498730 -0.628966
N13 4.310753 0.349468 0.264747
O14 3.561758 0.997946 0.979249
O15 5.529225 0.391406 0.277858

FS4.TS2'
N1 -1.606831 0.368256 -0.094482
C2 -0.593774 0.918091 0.092055
N3 0.472091 1.621800 0.407481
C4 2.042380 0.705614 0.085139
N5 1.542774 1.435256 -0.743469
H6 2.447671 0.069134 0.872775
O7 5.660846 -1.077792 -0.239068
N8 4.554084 -0.638891 0.056361
O9 3.929530 0.124783 -0.770793
O10 3.997682 -0.911356 1.156923
H11 -3.037193 -0.307785 -0.376441
O12 -3.862259 -0.835518 -0.685196
N13 -4.941777 -0.428788 0.037770
O14 -4.773435 0.432213 0.881909
O15 -5.982926 -0.983206 -0.244416

$OCHNNCN\cdot HNO_3$
N1 0.175240 -0.699734 -0.142166
C2 -0.946727 -0.453196 -0.258745
N3 -2.223254 -0.145130 -0.595179
C4 -4.366117 0.258711 -0.185402
N5 -3.038376 -0.085166 0.352346
H6 -4.376303 0.406184 -1.280051
O7 -5.295507 0.351471 0.549375
H8 2.079770 -0.819089 0.070473
O9 3.041442 -0.992129 0.187339
N10 3.656955 0.253956 0.061575
O11 2.926514 1.200358 -0.148356
O12 4.850006 0.229342 0.178946

NO_2^{-}
N1 0.000000 0.458837 0.000000
O2 1.071093 -0.200866 0.000000
O3 -1.071093 -0.200617 0.000000

FS4.TS2a'
N1 -1.111254 0.009270 0.110582
C2 -0.008534 -0.327260 0.292546
N3 1.171014 -0.773212 0.643918
C4 3.234461 -1.453688 0.010394
N5 2.144739 -0.579939 -0.252175
H6 2.997220 -2.176070 0.815810
O7 4.262916 -1.467038 -0.616490
N8 2.907693 1.115215 0.083925
O9 3.843458 1.496007 -0.574034
O10 2.217370 1.741491 0.848405
H11 -2.584407 0.393225 -0.180512
O12 -3.505323 0.798610 -0.453691
N13 -4.500948 -0.049975 -0.103264
O14 -4.202932 -1.089879 0.458612
O15 -5.621375 0.323186 -0.392031

$OCHN(NO_2)NCN^{-}\cdot HNO_3$
N1 1.073897 -0.124314 0.255654
C2 -0.022978 0.185462 0.522588
N3 -1.183541 0.579590 0.962716
C4 -3.046574 1.466480 -0.204941
N5 -2.225873 0.361491 0.067058
H6 -2.461440 2.366125 0.043008
O7 -4.175419 1.487084 -0.627133

N8 -2.795819 -0.990651 0.017122
O9 -3.687710 -1.177408 -0.788886
O10 -2.274753 -1.811824 0.742024
H11 2.489536 -0.415809 -0.134494
O12 3.423503 -0.767863 -0.492896
N13 4.409660 0.089029 -0.159996
O14 4.122312 1.083903 0.486192
O15 5.522185 -0.222392 -0.545835

FS4.TS2b'
N1 1.173542 -0.278475 -0.262584
C2 0.054960 -0.570674 -0.079632
N3 -1.126973 -1.034857 0.197492
C4 -2.819041 1.345138 0.508025
N5 -2.148824 -0.177554 -0.054494
H6 -2.854589 1.170421 1.588921
O7 -2.615062 2.364985 -0.069155
N8 -3.349901 -0.667283 -0.150955
O9 -4.171275 0.382971 0.030326
O10 -3.727313 -1.818716 -0.279142
H11 2.633157 0.106956 -0.486048
O12 3.574958 0.459943 -0.787695
N13 4.527660 0.032455 0.070449
O14 4.189507 -0.668435 1.009564
O15 5.658859 0.398732 -0.187972

[ONNNCN]$^{\bullet-}$·HNO$_3$
N1 -0.161744 -0.181625 0.004770
C2 0.997658 -0.028498 0.036417
N3 2.258594 0.301546 0.071068
N4 3.106243 -0.738678 0.088175
N5 4.380296 -0.388610 0.133723
O6 4.718119 0.753887 -0.235446
H7 -1.687460 -0.492239 -0.050975
O8 -2.648119 -0.887785 -0.106217
N9 -3.560786 0.109490 -0.006142
O10 -3.155895 1.251507 0.121443
O11 -4.721194 -0.249063 -0.055866

HCO$_2^{\bullet}$
C1 0.000029 0.433109 -0.000001
H2 -0.000025 1.530982 0.000002
O3 1.044221 -0.258107 0.000000
O4 -1.044240 -0.258097 0.000000

$^{\bullet}$NNCN·HNO$_3$
N1 1.096594 -0.548313 -0.085627
C2 2.210691 -0.249130 -0.098201
N3 3.515702 0.071976 -0.350396
N4 4.347404 0.397665 0.425728
H5 -0.818640 -0.781863 0.019006
O6 -1.767582 -1.032484 0.079942
N7 -2.470277 0.172785 0.016318
O8 -1.804839 1.181925 -0.091073
O9 -3.661512 0.052791 0.077135

NO
N1 0.000000 0.000000 -0.612285
O2 0.000000 0.000000 0.535749

HCO$_2^-$
C1 -0.000190 0.314526 0.000001
H2 0.002101 1.453693 -0.000001
O3 1.137559 -0.208962 0.000000
O4 -1.137679 -0.208644 0.000000

Cartesian coordinates for the structures in Figure 2a, calculated at B3LYP/ 6-311++G(d,p)

$DCBH^-$
B1 0.000000 0.000000 0.916166
C2 0.000000 1.316283 0.026260
C3 0.000000 -1.316283 0.026260
N4 0.000000 2.304968 -0.580606
N5 0.000000 -2.304968 -0.580606
H6 0.992485 0.000000 1.616267
H7 -0.992485 0.000000 1.616267

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$NCBH_2CN^-\cdot HNO_3$
C1 -4.067338 -0.179653 0.000235
N2 -4.875168 -1.010628 0.000139
C3 -1.525845 0.440972 0.000188
N4 -0.425864 0.082503 0.000059
H5 1.046741 -0.421507 -0.000122
N6 2.980964 -0.047117 -0.000212
O7 1.956005 -0.932998 -0.000266
O8 4.090617 -0.543439 -0.000374
O9 2.715856 1.142527 -0.000011
B10 -3.009220 0.999147 0.000377
H11 -3.150505 1.678086 -0.992502
H12 -3.150383 1.677738 0.993511

F2.TS0
N1 1.828497 -0.467176 0.027470
O2 2.826619 -0.700696 -0.674926
O3 1.921104 -0.110523 1.215508
O4 0.657551 -0.591626 -0.501910
H5 0.094294 2.804490 0.717010
C6 -2.675915 -0.538293 0.038448
N7 -3.301776 -1.278270 0.672186
C8 -0.616991 1.084408 -0.179049
N9 0.088678 1.890091 0.310950
B10 -1.925949 0.511438 -0.866561
H11 -1.642248 0.062372 -1.944982
H12 -2.614864 1.509496 -0.979240

$HNC(-ONO_2)BH_2CN^-$
N1 1.759691 -0.472452 -0.084163
O2 2.534111 -0.040932 -0.896406
O3 1.983075 -1.061713 0.937758
O4 0.353004 -0.351018 -0.444511
H5 -0.113557 2.382615 1.046368
C6 -2.677093 -0.362240 -0.070584
N7 -3.347746 -1.274928 0.180270
C8 -0.273676 0.814211 0.062148
N9 0.455910 1.597969 0.739931
B10 -1.818512 0.921744 -0.424841
H11 -1.826296 1.081632 -1.629317
H12 -2.299474 1.890389 0.130772

F2.TS1
N1 -2.473939 -0.033213 0.116236
O2 -3.125751 0.374093 -0.829374
O3 -2.931200 -0.623120 1.079068
O4 -0.393284 0.734827 0.295202
H5 1.459429 -1.371776 -1.088829
C6 3.178510 0.116109 0.197287
N7 4.025366 -0.661801 0.351682
C8 0.403972 -0.007164 -0.232955
N9 0.515024 -1.099354 -0.843664
B10 2.065421 1.174938 -0.033025
H11 1.865172 1.907775 0.881776
H12 1.990124 1.609818 -1.142763

HNCO
C1 -0.044851 0.021878 -0.000210
N2 1.158127 -0.122263 0.000066
O3 -1.210324 0.013896 0.000085
H4 1.844813 0.613402 0.000122

BH_2CN
C1 0.185555 0.000002 -0.000012
N2 1.343480 0.000001 0.000008
B3 -1.338863 0.000001 -0.000010
H4 -1.911667 -1.036716 0.000034
H5 -1.911710 1.036693 0.000034

NO_2^-
N1 0.000000 0.458837 0.000000
O2 1.071093 -0.200866 0.000000
O3 -1.071093 -0.200617 0.000000

F2.TS2
N1 -2.116743 -0.173038 0.193896
O2 -3.201950 -0.189498 0.743033
O3 -1.496700 -1.147860 -0.169755

O4 -0.594006 1.502711 -0.513917
H5 0.756758 -1.186107 -0.762089
C6 2.749607 -0.160190 0.400608
N7 3.558083 -0.976260 0.231259
C8 0.380204 0.715188 -0.392811
N9 0.194496 -0.422185 -1.154912
B10 1.618363 0.933864 0.624815
H11 1.183560 0.820393 1.757104
H12 2.079407 2.043956 0.467537

ONO-NHC(O)BH$_2$CN$^-$
N1 -2.100511 -0.470509 0.549527
O2 -3.258696 -0.540757 0.400907
O3 -1.425544 -0.527885 -0.751097
O4 -0.388944 1.850760 0.017361
H5 0.437568 -1.154702 -0.326002
C6 2.682072 -0.449878 0.186404
N7 3.144452 -1.515584 0.199287
C8 0.403913 0.928874 -0.106501
N9 -0.060256 -0.315035 -0.598067
B10 2.010103 0.990905 0.178351
H11 2.178749 1.513953 1.258664
H12 2.516930 1.663197 -0.696425

F2.TS2a
N1 2.462570 -0.650837 -0.650025
O2 3.579081 -0.777438 -0.331074
O3 1.344146 0.170697 0.975072
O4 -0.131724 2.115600 -0.277911
H5 -0.331334 -0.871709 0.674529
C6 -2.542025 -0.873562 -0.174199
N7 -2.734746 -2.007078 -0.006370
C8 -0.695532 1.068321 -0.018245
N9 -0.018573 0.088489 0.775234
B10 -2.231793 0.669333 -0.401358
H11 -2.406729 0.940945 -1.569674
H12 -2.974420 1.330643 0.296036

[ONHC(O)BH$_2$CN]$^{\bullet-}$
N1 -2.100511 -0.470509 0.549527
O2 -3.258696 -0.540757 0.400907
O3 -1.425544 -0.527885 -0.751097
O4 -0.388944 1.850760 0.017361
H5 0.437568 -1.154702 -0.326002
C6 2.682072 -0.449878 0.186404
N7 3.144452 -1.515584 0.199287
C8 0.403913 0.928874 -0.106501
N9 -0.060256 -0.315035 -0.598067
B10 2.010103 0.990905 0.178351
H11 2.178749 1.513953 1.258664
H12 2.516930 1.663197 -0.696425

NO
N1 0.000000 0.000000 -0.612285
O2 0.000000 0.000000 0.535749

F2.TS2b
N1 -2.859095 0.091694 0.294670
O2 -3.981950 0.241411 -0.160706
O3 -1.919591 0.480578 -0.516940
O4 0.688248 -1.754057 -0.409564
H5 0.059793 1.227099 0.190957
C6 3.050997 0.455021 -0.029355
N7 3.802983 0.786970 -0.847182
C8 0.622962 -0.677614 0.098252
N9 -0.187949 0.274294 0.422549
B10 2.047810 0.055428 1.101280
H11 2.292849 -0.961838 1.682802
H12 1.779329 0.978992 1.813877

OCNBH$_2$CN$^-$
B1 -0.775457 1.010498 -0.000029
H2 -0.902898 1.698144 0.995772
H3 -0.902764 1.697996 -0.995950
N4 0.602633 0.333526 0.000123
C5 -1.943023 -0.083600 -0.000031
C6 1.706561 -0.073038 -0.000058
O7 2.831038 -0.496130 -0.000009
N8 -2.823573 -0.839206 0.000011

HONO
H1 1.720096 0.440472 0.000101
N2 -0.179880 0.486515 -0.000014
O3 -1.102769 -0.225490 0.000011
O4 1.045152 -0.255270 -0.000011

F2.TS3
C1 -0.305546 0.464234 0.020737
N2 0.562381 1.087928 -0.719356
C3 -2.917960 -0.189398 0.015935
N4 -3.719807 -1.021083 -0.087184
H5 0.301236 1.876184 -1.302187
O6 0.124228 -0.515502 0.690680
N7 2.000816 -0.243661 -0.007870
O8 2.684520 0.264197 0.833051
O9 2.268251 -1.073817 -0.826191
B10 -1.885237 0.998539 0.139876
H11 -1.958439 1.508765 1.236584
H12 -2.095296 1.812027 -0.733256

O_2N-NHC(O)BH_2CN^-
C1 0.423217 0.195232 0.060797
N2 -0.860962 -0.523482 0.345103
C3 3.052821 -0.246679 -0.030739
N4 4.126419 0.181653 -0.118277
H5 -0.816867 -1.521542 0.177218
O6 0.406680 1.376058 -0.154410
N7 -2.120692 -0.073246 0.021185
O8 -2.371944 1.111781 0.153541
O9 -2.926063 -0.936191 -0.360208
B10 1.622095 -0.897611 0.097061
H11 1.535342 -1.521128 1.137644
H12 1.432087 -1.668259 -0.827979

F2.TS3a
C1 0.537722 0.618515 0.407512
N2 -0.274752 -0.237043 -0.064619
C3 3.022735 -0.443732 -0.260240
N4 3.868288 -0.240728 -1.026733
H5 -0.512771 -1.089457 0.427556
O6 0.811046 1.766659 0.564689
N7 -2.459665 -0.121037 -0.209813
O8 -3.218389 0.696266 -0.706262
O9 -2.843031 -1.179473 0.297225
B10 1.922871 -0.766795 0.786163
H11 2.083544 -0.311727 1.882099
H12 1.518020 -1.889506 0.738841

$OCNBH_2CN^-$
B1 -0.775457 1.010498 -0.000029
H2 -0.902898 1.698144 0.995772
H3 -0.902764 1.697996 -0.995950
N4 0.602633 0.333526 0.000123
C5 -1.943023 -0.083600 -0.000031
C6 1.706561 -0.073038 -0.000058
O7 2.831038 -0.496130 -0.000009
N8 -2.823573 -0.839206 0.000011

HONO
H1 1.720096 0.440472 0.000101
N2 -0.179880 0.486515 -0.000014
O3 -1.102769 -0.225490 0.000011
O4 1.045152 -0.255270 -0.000011

F2.TS3b
N1 2.204800 -0.171948 -0.261567
N2 0.133211 -0.653139 -0.041675
H3 0.620328 -1.160695 0.704281
C4 -0.531781 0.541039 0.498135
O5 -0.058873 1.636499 0.613287
B6 -1.828624 -0.325798 0.767664
H7 -1.061796 -1.352538 0.188405
H8 -2.039506 -0.618956 1.908485
C9 -3.026965 -0.244196 -0.207357
N10 -3.941522 -0.192564 -0.918476
O11 2.847804 -0.861148 0.544844
O12 2.736211 0.487609 -1.137148

***cyclic*-NH_2-[C-O-BH]-CN**
N1 2.032173 -0.780013 -0.008183
H2 2.755041 -0.555372 -0.681365
C3 0.979284 -0.002860 0.128875
O4 0.727475 1.066092 -0.497162
B5 -0.361447 0.484748 0.676919
H6 2.115150 -1.624858 0.534425
H7 -0.394479 1.145157 1.659750
C8 -1.668989 -0.098097 0.090719
N9 -2.653607 -0.550224 -0.311484

NO_2^-
N1 0.000000 0.458837 0.000000
O2 1.071093 -0.200866 0.000000
O3 -1.071093 -0.200617 0.000000

F2.TS4
C1 3.209220 -0.554604 -0.078395
N2 3.975730 -1.138418 -0.720724
C3 1.096407 0.983673 0.269472
N4 0.447675 1.953548 -0.177525
H5 -0.537567 1.685731 -0.361446
N6 -2.285218 -0.371971 -0.035078
O7 -2.238041 0.804346 -0.496370
O8 -3.356336 -0.998471 -0.010927
O9 -1.222377 -0.909288 0.406176
B10 2.273371 0.270289 0.825728
H11 0.519203 -0.043348 0.423483
H12 2.384480 0.156956 2.005121

$O_3NH{\cdot}NCHBHCN^-$
C1 -3.760788 0.057854 0.000089
N2 -4.734330 -0.568485 0.000185
C3 -1.082104 0.439740 0.000011
N4 -0.879210 -0.833004 -0.000202
H5 0.144897 -1.013639 -0.000232
N6 2.712920 -0.007436 -0.000007
O7 2.065065 -1.099704 -0.000238
O8 3.959365 -0.023574 -0.000005
O9 2.082857 1.084554 0.000219
B10 -2.529810 0.985206 -0.000006
H11 -0.222374 1.121306 0.000139

H12 -2.770069 2.153007 -0.000105

HNCHBH(-ONO_2)CN^-
N1 -1.694217 -0.285538 0.008757
O2 -0.416388 -0.614404 -0.248065
O3 -1.936823 0.648565 0.757740
O4 -2.528603 -0.978068 -0.557330
B5 0.704813 0.135913 0.471956
C6 2.068210 -0.691691 0.277617
C7 0.894859 1.605603 -0.131785
N8 2.189940 -1.885450 -0.171484
N9 1.094210 2.667701 -0.549859
H10 2.966290 -0.140378 0.620889
H11 0.484292 0.230199 1.659074
H12 3.171923 -2.178599 -0.145404

F2.TS5
C1 -3.041363 -0.057911 -0.000026
N2 -4.186329 0.127668 0.000028
C3 -1.277752 0.160084 -0.000021
N4 -0.863987 1.306368 0.000106
H5 0.200192 1.299502 0.000080
N6 2.298920 -0.059148 0.000023
O7 1.889322 1.151524 -0.000103
O8 3.516820 -0.292922 -0.000133
O9 1.455796 -0.992953 0.000311
B10 -1.389544 -1.336082 -0.000195
H11 -1.486755 -1.890886 1.045439
H12 -1.486760 -1.890646 -1.045959

HNC(CN)BH_2(-ONO_2)$^-$
C1 2.672642 -0.084698 0.127824
N2 3.738496 -0.467739 0.363050
C3 1.301368 0.312256 -0.188803
N4 1.090396 1.581271 -0.182404
H5 0.108225 1.738136 -0.427551
N6 -1.968526 -0.097111 0.166237
O7 -1.573224 -0.165717 1.319158
O8 -3.106317 0.200059 -0.178262
O9 -1.117440 -0.353895 -0.846195
B10 0.298059 -0.907466 -0.543958
H11 0.635258 -1.389403 -1.605848
H12 0.275445 -1.735275 0.333264

F2.TS6
C1 2.554442 -0.799280 -0.108330
N2 3.176377 -1.537508 -0.751792
C3 1.141147 1.345698 0.245737
N4 0.547570 2.316605 -0.204470
H5 -0.433436 2.119432 -0.446900
N6 -1.915316 -0.372688 -0.037028
O7 -2.863904 -1.149536 -0.053050
O8 -1.005090 -0.537849 0.897307
O9 -1.775307 0.556372 -0.848121
B10 1.752211 0.160828 0.798294
H11 0.154016 -0.055502 0.629689
H12 1.838818 0.056672 1.985237

HNCBH(·HNO_3)CN^-
C1 2.593450 -0.846444 -0.105779
N2 3.176632 -1.611408 -0.758883
C3 1.220283 1.313950 0.267922
N4 0.735416 2.366579 -0.166273
H5 -0.244063 2.276053 -0.462575
N6 -2.005897 -0.333150 -0.072397
O7 -3.016983 -1.005070 -0.026772
O8 -1.083282 -0.607760 0.884697
O9 -1.753364 0.546698 -0.881606
B10 1.838434 0.138916 0.806726
H11 -0.170829 -0.155484 0.638642
H12 1.826301 -0.045275 1.989756

O_2NO^-·HNC
C1 -3.391024 0.105517 0.000298
N2 -2.241831 -0.089586 0.000174
H3 -1.179023 -0.294118 0.000056
N4 1.217748 0.024541 -0.000098
O5 0.248887 -0.825755 -0.000139
O6 2.382922 -0.401788 -0.000260
O7 0.954910 1.242085 0.000101

BH_2(ONO_2)CN^-
B1 0.886347 0.764545 0.000056
H2 0.767843 1.428360 -1.003076
H3 0.767876 1.428271 1.003254
O4 -0.144845 -0.402884 0.000033
N5 -1.441669 -0.095121 -0.000006
O6 -1.783231 1.080440 -0.000047
O7 -2.208949 -1.053933 0.000002
C8 2.293689 0.024890 -0.000001
N9 3.351186 -0.450261 -0.000045

HNC
N1 0.000000 0.000000 0.429586
C2 0.000000 0.000000 -0.739365
H3 0.000000 0.000000 1.429086

Cartesian coordinates for the structures in Figure 2b, calculated at B3LYP/ 6-311++G(d,p)

$DCBH^-$
B1 0.000000 0.000000 0.916166
C2 0.000000 1.316283 0.026260
C3 0.000000 -1.316283 0.026260
N4 0.000000 2.304968 -0.580606
N5 0.000000 -2.304968 -0.580606
H6 0.992485 0.000000 1.616267
H7 -0.992485 0.000000 1.616267

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$O_3NH \cdot NCBH_2CN^- \cdot HNO_3$
C1 -1.303627 1.013566 0.022980
N2 -2.284749 0.402570 0.039911
C3 1.303620 1.013386 -0.021348
N4 2.284662 0.402270 -0.038610
H5 3.649791 -0.432184 -0.068845
N6 5.605634 -0.470861 0.007495
O7 4.416161 -1.120153 -0.110626
O8 6.584457 -1.186944 -0.028749
O9 5.587189 0.739901 0.135955
B10 0.000062 1.908702 0.001078
H11 -0.016643 2.596557 -0.992104
H12 0.016886 2.595942 0.994688
H13 -3.649875 -0.431883 0.070144
O14 -4.416247 -1.119815 0.112509
N15 -5.605622 -0.470894 -0.008566
O16 -5.587114 0.739571 -0.139802
O17 -6.584434 -1.186968 0.028128

F2.TS0'
N1 3.470811 -1.092930 0.028891
O2 4.351966 -1.640388 -0.648133
O3 3.475496 -1.102853 1.270999
O4 2.512465 -0.473596 -0.587380
H5 3.485439 2.264342 1.571416
C6 -0.268619 0.935708 -0.602245
N7 -1.254612 0.350105 -0.467655
C8 2.216756 1.461981 0.110838
N9 3.083334 1.670447 0.876609
B10 0.996801 1.843533 -0.825562
H11 1.364695 1.787714 -1.969769
H12 0.721452 2.981711 -0.509395
H13 -2.654814 -0.404122 -0.300400
O14 -3.479119 -1.022196 -0.263637
N15 -4.548473 -0.312352 0.182981
O16 -4.382802 0.862186 0.460728
O17 -5.583883 -0.940696 0.259750

$HNC(-ONO_2)BH_2CN^- \cdot HNO_3$
B1 1.062458 1.886344 -0.528948
C2 -0.259015 1.063791 -0.252731
C3 2.353619 1.217109 0.158931
N4 -1.258199 0.513512 -0.061141
N5 3.179490 1.619900 0.991765
H6 1.240740 1.930302 -1.726113
H7 0.929480 2.991426 -0.063693
H8 -2.611261 -0.222619 0.222019
O9 -3.404390 -0.831607 0.508933
N10 -4.570456 -0.300310 0.066342
O11 -5.566937 -0.930915 0.359745
O12 -4.526030 0.736752 -0.572030
O13 2.472142 -0.219199 -0.509334
H14 3.971083 1.001564 1.158921
N15 3.439624 -1.118257 -0.160767
O16 3.135846 -2.281652 -0.306486
O17 4.521473 -0.701094 0.239548

F2.TS1'
N1 -4.807906 -0.537495 0.189265
O2 -5.707133 0.063398 -0.378062
O3 -4.952813 -1.582668 0.803046
O4 -2.829313 0.614670 0.494506
H5 -0.886416 -0.067648 -1.863080
C6 0.655490 0.997039 0.202278
N7 1.628653 0.374119 0.125084
C8 -2.056804 0.389934 -0.395215
N9 -1.797064 -0.222203 -1.450910
B10 -0.625173 1.859055 0.295770
H11 -0.948171 2.186535 1.387933
H12 -0.855495 2.560636 -0.637445
H13 3.086471 -0.436564 0.043714
O14 3.873374 -1.073473 -0.026206
N15 5.025041 -0.338771 0.048215
O16 4.921154 0.866522 0.175647
O17 6.044268 -0.987152 -0.023173

HNCO
C1 -0.044851 0.021878 -0.000210
N2 1.158127 -0.122263 0.000066
O3 -1.210324 0.013896 0.000085

H4 1.844813 0.613402 0.000122

$BH_2CN \cdot HNO_3$
B1 4.228333 0.284791 0.000080
C2 2.749630 -0.112779 -0.000009
N3 1.632756 -0.405990 -0.000074
H4 -0.220847 -0.712413 -0.000082
O5 -1.159579 -1.018330 -0.000039
N6 -1.932423 0.139585 -0.000005
O7 -3.116740 -0.055602 0.000113
O8 -1.332295 1.194961 -0.000067
H9 4.774042 0.430920 -1.039170
H10 4.773944 0.430816 1.039395

NO_2^-
N1 0.000000 0.458837 0.000000
O2 1.071093 -0.200866 0.000000
O3 -1.071093 -0.200617 0.000000

F2.TS2'
N1 -4.013575 -0.846608 0.220695
O2 -5.009794 -1.272793 0.769287
O3 -3.017168 -1.489219 -0.032092
O4 -3.312153 1.241853 -0.691186
H5 -0.949386 -0.646268 -0.593147
C6 0.369536 1.396559 0.378594
N7 1.485049 1.100007 0.281561
C8 -2.110533 0.955979 -0.470653
N9 -1.755528 -0.233726 -1.075588
B10 -1.154825 1.799804 0.525224
H11 -1.493192 1.543995 1.664891
H12 -1.265193 2.983697 0.305522
H13 3.021069 0.752380 0.192441
O14 4.056608 0.711923 0.163930
O15 3.593059 -1.432775 -0.107388
O16 5.655076 -0.741143 -0.048554
N17 4.452880 -0.575505 -0.008875

$ONO\text{-}NHC(O)BH_2CN^- \cdot HNO_3$
C1 -2.109745 0.501280 -0.412429
N2 -3.268218 0.703779 0.391609
C3 0.516290 0.784608 -0.098959
N4 1.570470 0.315154 -0.180993
O5 -2.154775 -0.311431 -1.316596
H6 -3.324688 1.569006 0.913298
H7 2.981408 -0.311898 -0.285212
O8 3.853053 -0.866363 -0.449434
N9 4.905433 -0.256197 0.143573
O10 5.971742 -0.826760 0.016088
O11 4.707138 0.787782 0.741356
O12 -4.514477 0.395692 -0.149407
N13 -4.987409 -0.970066 0.202452
O14 -4.266628 -1.576340 0.880316
B15 -0.891693 1.475443 0.049191
H16 -0.925210 2.445128 -0.683013
H17 -1.022667 1.835890 1.202231

F2.TS2a′
No converged structure was located. The energy was determined from a relaxed PES scan.

$[ONHC(O)BH_2CN]^{\bullet -} \cdot HNO_3$
C1 2.963287 -0.158748 0.089538
N2 4.274023 0.421401 -0.183144
C3 0.375061 0.435824 0.154973
N4 -0.720450 0.069191 0.098367
H5 4.302980 1.436347 -0.304686
O6 2.888859 -1.362872 0.202015
B7 1.842184 1.001079 0.233594
H8 1.992857 1.540329 1.313415
H9 1.983550 1.836546 -0.638975
O10 5.371071 -0.216097 -0.267049
H11 -2.194376 -0.420377 0.023623
O12 -3.112150 -0.914825 -0.025709
N13 -4.118898 -0.009774 -0.063335
O14 -5.236519 -0.484314 -0.123313
O15 -3.832355 1.174805 -0.034898

NO
N1 0.000000 0.000000 -0.612285
O2 0.000000 0.000000 0.535749

F2.TS2b'
N1 -5.230909 -0.356839 -0.253058
O2 -6.205140 -1.093392 -0.215010
O3 -4.099342 -0.993325 -0.235720
O4 -1.851618 0.806240 1.759785
H5 -2.214301 -0.227683 -1.147247
C6 0.621866 0.892100 -0.273465
N7 1.609752 0.321827 -0.082621
C8 -1.918044 0.714151 0.578580
N9 -2.610902 0.380573 -0.444325
B10 -0.696587 1.669931 -0.581343
H11 -0.826944 2.704147 -0.000720
H12 -0.935488 1.699128 -1.750123
H13 3.066459 -0.423773 0.171775
O14 3.863538 -1.010878 0.407554
N15 4.995883 -0.411150 -0.067308
O16 6.020850 -1.016587 0.153739
O17 4.874650 0.647960 -0.653657

$OCNBH_2CN^{-}\cdot HNO_3$
C1 4.341204 -0.412121 0.000009
N2 3.381464 0.270993 -0.000043
C3 0.848425 0.674455 -0.000021
N4 -0.223192 0.237824 -0.000006
O5 5.305145 -1.122300 0.000057
B6 2.300495 1.346881 -0.000042
H7 2.368369 2.038009 0.995700
H8 2.368346 2.037992 -0.995797
H9 -1.647686 -0.379709 -0.000011
O10 -2.513177 -0.964614 -0.000031
N11 -3.607732 -0.166985 0.000011
O12 -4.672732 -0.753360 -0.000033
O13 -3.442118 1.040584 0.000089

HONO
H1 1.720096 0.440472 0.000101
N2 -0.179880 0.486515 -0.000014
O3 -1.102769 -0.225490 0.000011
O4 1.045152 -0.255270 -0.000011

F2.TS3'
C1 -2.191394 0.718837 -0.020329
N2 -3.235823 1.062960 0.673444
C3 0.475995 0.902131 -0.162689
N4 1.497745 0.360179 -0.145912
H5 -3.264376 1.917020 1.220334
O6 -2.265823 -0.389893 -0.627406
N7 -4.127842 -0.700142 0.055389
O8 -4.917819 -0.494741 -0.815449
O9 -4.112599 -1.513846 0.927748
B10 -0.876307 1.713988 -0.174060
H11 -0.995306 2.262831 -1.245666
H12 -0.852754 2.517189 0.729170
H13 2.882735 -0.370411 -0.137288
O14 3.705510 -1.006365 -0.167738
N15 4.838221 -0.296959 0.058555
O16 5.864375 -0.947655 0.043081
O17 4.738547 0.901918 0.253706

O_2N-NHC(O)$BH_2CN^{-}\cdot HNO_3$
C1 -2.023018 0.092231 0.234516
N2 -3.350819 -0.563040 0.221088
C3 0.565866 -0.472146 0.242213
N4 1.653019 -0.095303 0.129871
H5 -3.347092 -1.527901 -0.085898
O6 -1.936863 1.288315 0.147225
N7 -4.544096 0.026872 -0.148198
O8 -4.736910 1.190884 0.147654
O9 -5.346574 -0.708924 -0.736562
B10 -0.888333 -1.054719 0.402906
H11 -1.003213 -1.536434 1.510119
H12 -1.057902 -1.925426 -0.426920
H13 3.135409 0.416594 -0.020796
O14 4.036231 0.919502 -0.130214
N15 5.057532 0.026249 -0.119197
O16 6.164582 0.510643 -0.242298
O17 4.788025 -1.155070 0.009651

F2.TS3a'
C1 2.000585 0.452143 0.886917
N2 2.588993 0.121069 -0.183790
C3 -0.561084 0.863045 -0.071831
N4 -1.572529 0.304425 -0.029899
H5 3.026047 0.795809 -0.804606
O6 1.785647 0.269653 2.040281
N7 4.682038 -0.597337 -0.392220
O8 5.347042 -1.526160 0.035204
O9 5.112357 0.220012 -1.215364
B10 0.775862 1.647878 -0.158750
H11 0.920269 2.512104 0.653617
H12 1.112442 1.896557 -1.274188
H13 -3.043669 -0.445366 0.022590
O14 -3.856308 -1.054894 0.096607
N15 -4.973098 -0.322460 -0.188509
O16 -6.012944 -0.940889 -0.133879
O17 -4.826946 0.853589 -0.464506

$OCNBH_2CN^{-}\cdot HNO_3$
C1 4.341204 -0.412121 0.000009
N2 3.381464 0.270993 -0.000043
C3 0.848425 0.674455 -0.000021
N4 -0.223192 0.237824 -0.000006
O5 5.305145 -1.122300 0.000057
B6 2.300495 1.346881 -0.000042
H7 2.368369 2.038009 0.995700
H8 2.368346 2.037992 -0.995797
H9 -1.647686 -0.379709 -0.000011
O10 -2.513177 -0.964614 -0.000031
N11 -3.607732 -0.166985 0.000011
O12 -4.672732 -0.753360 -0.000033
O13 -3.442118 1.040584 0.000089

HONO
H1 1.720096 0.440472 0.000101
N2 -0.179880 0.486515 -0.000014
O3 -1.102769 -0.225490 0.000011
O4 1.045152 -0.255270 -0.000011

F2.TS3b′
N1 -4.418546 -0.687654 -0.306488
N2 -2.465057 0.119959 -0.620930
H3 -3.099534 0.701115 -1.179449
C4 -2.084888 0.817887 0.615970
O5 -2.680493 0.819948 1.654440
B6 -0.823674 1.417882 -0.129591
H7 -1.344006 0.626519 -1.204340
H8 -0.850818 2.574574 -0.421422
C9 0.553453 0.746477 0.048467
N10 1.597436 0.261879 0.171445
O11 -5.209390 -0.098740 -1.055066
O12 -4.714711 -1.678710 0.333318
H13 3.108423 -0.379054 0.317577
O14 3.962819 -0.898555 0.514903
N15 4.998908 -0.291558 -0.135340
O16 6.076145 -0.822984 0.019695
O17 4.753597 0.701901 -0.793769

***cyclic*-NH_2-[C-O-BH]-CN·HNO_3**
N1 3.497973 -1.646289 0.159764
H2 3.981879 -2.094352 -0.609765
C3 3.151086 -0.384020 0.089087
O4 3.359011 0.426577 -0.864688
B5 2.558142 0.969219 0.480886
H6 3.245947 -2.198527 0.964721
H7 3.163121 1.731553 1.154691
C8 1.035414 1.188211 0.260222
N9 -0.101753 1.329128 0.134359
H10 -1.848129 1.029552 -0.026467
O11 -2.837174 0.959258 -0.126835
N12 -3.148447 -0.383938 -0.030011
O13 -2.224774 -1.155568 0.146411
O14 -4.320430 -0.634239 -0.133920

NO_2^-
N1 0.000000 0.458837 0.000000
O2 1.071093 -0.200866 0.000000
O3 -1.071093 -0.200617 0.000000

F2.TS3c'
C1 -1.492415 1.240773 -0.213536
N2 -1.266125 -0.150434 0.045327
C3 1.179190 1.624770 0.202564
N4 2.133451 1.722181 0.912100
O5 -2.606316 1.713765 -0.259300
H6 -0.346370 -0.530585 -0.211843
N7 -2.242262 -1.131133 0.111749
O8 -1.887560 -2.258996 -0.233009
O9 -3.350336 -0.832287 0.522687
H10 2.349612 2.465373 1.557959
O11 3.447292 -1.039873 -0.748258
N12 2.388439 -0.897739 -0.136393
O13 2.182305 -1.347134 0.993959
O14 1.428563 -0.208873 -0.715562
B15 -0.141861 2.100585 -0.508202
H16 -0.276946 3.219376 -0.055118
H17 0.056250 2.136716 -1.697779

O_2N-NHC(O)BH_2C(ONO_2)NH^-
C1 1.115334 0.045252 0.296513
N2 2.336876 0.306309 -0.513394
C3 -1.463726 0.826993 0.371950
N4 -2.293227 1.177130 1.262278
O5 1.067003 -0.918134 1.014288
H6 2.403571 1.249360 -0.876323
N7 3.605079 -0.169739 -0.251913
O8 4.537435 0.598008 -0.530559
O9 3.730152 -1.293620 0.199607
H10 -1.835525 1.824868 1.898225
O11 -1.928890 -0.084815 -0.606086
N12 -3.319795 -0.494293 -0.421792
O13 -4.125660 0.161649 -1.025843
O14 -3.483283 -1.481574 0.238691
B15 0.061305 1.258177 0.066114
H16 0.379007 2.129550 0.857996
H17 0.160178 1.683896 -1.068286

F2.TS3d'
C1 -1.560213 -1.229306 -0.024503
N2 -1.663100 0.179121 0.347560
C3 1.199487 -0.917493 0.109506
N4 2.345139 -1.378705 -0.274092
O5 -2.510682 -1.809865 -0.495111
H6 -0.783786 0.692719 0.403401
N7 -2.710725 1.027694 0.060408
O8 -2.413262 2.219793 -0.081503
O9 -3.840403 0.573480 -0.002648
H10 2.451743 -2.360962 -0.504345
O11 1.145637 0.335166 0.349725
N12 3.063007 0.638284 -0.085631
O13 3.171256 1.144486 -1.158973
O14 3.697647 0.762228 0.915738
B15 -0.125966 -1.899051 0.351876
H16 -0.129855 -2.103192 1.550703
H17 0.014296 -2.919577 -0.274697

O_2N·NHC(O)BH_2C(O)NH·NO_2^-
C1 1.488609 -1.188545 -0.033524
N2 1.907783 0.170212 0.290800

C3 -1.033147 -0.123838 0.017237
H4 1.173877 0.882368 0.237651
O5 2.290687 -2.013570 -0.404303
N6 3.155559 0.713512 0.065143
O7 4.136625 -0.006105 0.145967
O8 3.179241 1.925940 -0.175128
B9 -0.095461 -1.428356 0.224988
H10 -0.491073 -2.347864 -0.457698
H11 -0.222866 -1.720905 1.403891
N12 -2.409282 -0.534951 -0.209597
N13 -3.558258 0.221068 -0.049124
O14 -3.502800 1.423785 -0.215172
O15 -4.575596 -0.422451 0.231913
O16 -0.750117 1.058027 0.059698
H17 -2.610348 -1.511426 -0.035419

F2.TS4'
C1 0.612748 0.914249 0.298423
N2 1.623532 0.474751 -0.058079
C3 -1.828050 1.810591 -0.028788
N4 -2.786643 2.043586 -0.738534
H5 -3.472886 1.257664 -0.861119
N6 -4.243689 -1.002489 0.041596
O7 -4.577059 -0.173540 -0.864358
O8 -4.983483 -1.953065 0.321110
O9 -3.145238 -0.832967 0.654281
B10 -0.705519 1.525972 0.862257
H11 -1.721418 0.597412 0.584686
H12 -0.799504 1.767406 2.040849
H13 3.078074 -0.370402 -0.293414
O14 3.839568 -1.016279 -0.475173
N15 5.006316 -0.418355 -0.072437
O16 4.925467 0.706344 0.395269
O17 6.008060 -1.094673 -0.232118

O_3N^-·HNCHBHCN·HNO_3
C1 1.003882 0.722262 0.000080
N2 2.036346 0.206725 0.000102
C3 -1.682122 0.774966 0.000000
N4 -1.683850 -0.515406 0.000093
H5 -2.669113 -0.856684 0.000069
N6 -5.314082 -0.276433 -0.000032
O7 -4.501950 -1.254847 -0.000141
O8 -6.540255 -0.487142 -0.000079
O9 -4.860400 0.900346 0.000120
B10 -0.329690 1.512483 0.000033
H11 -2.635185 1.317157 -0.000074
H12 -0.215201 2.696851 0.000025
H13 3.623544 -0.511557 0.000094
O14 4.454463 -1.073066 0.000141
N15 5.529821 -0.215393 -0.000047
O16 5.296138 0.977380 -0.000232
O17 6.606528 -0.761172 -0.000005

HNCHBH(-ONO_2)CN^-·HNO_3
N1 3.034616 -1.317525 -0.018546
O2 2.746574 -0.032308 -0.318763
O3 2.390614 -1.883992 0.850728
O4 3.937227 -1.807755 -0.675642
B5 1.737921 0.707348 0.542266
C6 1.804922 2.273661 0.191534
C7 0.248662 0.184042 0.257657
N8 2.702681 2.853014 -0.512584
N9 -0.848096 -0.131381 0.076118
H10 0.999000 2.870550 0.660769
H11 1.952284 0.561415 1.723750
H12 2.537257 3.863870 -0.543420
H13 -2.367527 -0.559556 -0.165297
O14 -3.279758 -0.987298 -0.387280
N15 -4.271136 -0.113150 -0.070120
O16 -3.956633 0.964487 0.402357
O17 -5.395346 -0.510127 -0.297195

F2.TS5'
C1 -0.574538 0.010996 0.131848
N2 -1.717627 -0.179299 0.156427
C3 1.376344 -0.350901 -0.000208
N4 1.722456 -1.482291 -0.195380
H5 2.799599 -1.479136 -0.231974
N6 4.680140 0.146957 -0.027336
O7 4.382550 -1.080048 -0.219944
O8 5.861374 0.492711 -0.006221
O9 3.758930 1.001438 0.140792
B10 1.399297 1.139158 0.239988
H11 1.281556 1.849277 -0.701629
H12 1.353241 1.514989 1.363210
H13 -3.331184 -0.467592 0.228139
O14 -4.280993 -0.822448 0.354369
N15 -5.163257 0.127055 -0.073272
O16 -6.330491 -0.181812 0.029360
O17 -4.711684 1.170051 -0.507181

HNC(CN)BH_2(-ONO_2)$^-$·HNO_3
C1 0.293148 0.250994 0.277236
N2 1.404566 -0.055835 0.238257
C3 -1.129586 0.586631 0.246790
N4 -1.502784 1.380118 1.185896
H5 -2.505216 1.557125 1.070872
N6 -4.263463 -0.367846 -0.077376
O7 -3.792313 -1.199166 0.681491

O8 -5.448591 -0.085154 -0.180240
O9 -3.439092 0.334441 -0.886970
B10 -1.954209 -0.063857 -0.985734
H11 -1.584630 0.467404 -2.011824
H12 -1.804693 -1.260196 -1.027687
H13 3.016316 -0.509213 0.238992
O14 3.922842 -0.956157 0.321308
N15 4.875719 -0.077395 -0.116954
O16 6.010831 -0.494861 -0.062265
O17 4.505029 1.011537 -0.510149

F2.TS6'
C1 0.310220 0.747406 0.445094
N2 1.328157 0.277429 0.157303
C3 -1.906387 1.929207 -0.129987
N4 -2.726650 2.289741 -0.948486
H5 -3.431571 1.574493 -1.181282
N6 -3.747821 -1.081402 0.025605
O7 -4.271077 -2.179443 0.170918
O8 -3.078710 -0.581163 1.036179
O9 -3.825451 -0.422567 -1.027565
B10 -1.031712 1.368643 0.881904
H11 -2.189530 0.345749 0.729833
H12 -1.167669 1.695168 2.021154
H13 2.760865 -0.337065 -0.257692
O14 3.573099 -0.835426 -0.641177
N15 4.707633 -0.327352 -0.086138
O16 4.593764 0.568308 0.730625
O17 5.737654 -0.835978 -0.475253

HNCBH(·HNO$_3$)CN$^-$·HNO$_3$
C1 0.364221 0.945509 0.424168
N2 1.386740 0.519767 0.074926
C3 -1.927924 2.001410 -0.006560
N4 -2.739503 2.490968 -0.794060
H5 -3.437131 1.827301 -1.148329
N6 -3.751433 -1.201006 -0.046213
O7 -4.326002 -2.253843 0.118881
O8 -2.976423 -0.797672 1.001816
O9 -3.799880 -0.485272 -1.033066
B10 -0.968380 1.501993 0.933199
H11 -2.424808 0.024096 0.716395
H12 -1.158622 1.585026 2.109456
H13 2.765688 -0.025081 -0.416041
O14 3.594888 -0.416887 -0.908619
N15 4.663696 -0.415637 -0.074748
O16 4.511010 0.008956 1.057265
O17 5.691717 -0.850465 -0.555334

BH$_2$CN·HNO$_3$
B1 4.228333 0.284791 0.000080
C2 2.749630 -0.112779 -0.000009
N3 1.632756 -0.405990 -0.000074
H4 -0.220847 -0.712413 -0.000082
O5 -1.159579 -1.018330 -0.000039
N6 -1.932423 0.139585 -0.000005
O7 -3.116740 -0.055602 0.000113
O8 -1.332295 1.194961 -0.000067
H9 4.774042 0.430920 -1.039170
H10 4.773944 0.430816 1.039395

O$_2$NO$^-$·HNC
C1 -3.391024 0.105517 0.000298
N2 -2.241831 -0.089586 0.000174
H3 -1.179023 -0.294118 0.000056
N4 1.217748 0.024541 -0.000098
O5 0.248887 -0.825755 -0.000139
O6 2.382922 -0.401788 -0.000260
O7 0.954910 1.242085 0.000101

BH$_2$(-ONO$_2$)CN$^-$·HNO$_3$
B1 1.810268 0.934766 0.000047
H2 1.988590 1.580718 1.003320
H3 1.988576 1.580809 -1.003169
O4 4.624906 -1.265084 -0.000068
N5 3.993903 -0.216366 -0.000017
O6 2.660492 -0.354362 -0.000017
O7 4.476866 0.906360 0.000033
H8 -2.290852 -0.439142 0.000026
O9 -3.197428 -0.941643 0.000033
N10 -4.213755 -0.041674 -0.000011
O11 -3.932528 1.143571 -0.000049
O12 -5.327555 -0.525945 -0.000007
C13 0.316699 0.386619 0.000034
N14 -0.790986 0.055311 0.000028

HNC
N1 0.000000 0.000000 0.429586
C2 0.000000 0.000000 -0.739365
H3 0.000000 0.000000 1.429086

Cartesian coordinates for the structures in Figure 3a, calculated at B3LYP/ 6-311++G(d,p)

$DCBH^-$
B1 0.000000 0.000000 0.916166
C2 0.000000 1.316283 0.026260
C3 0.000000 -1.316283 0.026260
N4 0.000000 2.304968 -0.580606
N5 0.000000 -2.304968 -0.580606
H6 0.992485 0.000000 1.616267
H7 -0.992485 0.000000 1.616267

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$NCBH_2CN^-\cdot HNO_3$
C1 -4.067338 -0.179653 0.000235
N2 -4.875168 -1.010628 0.000139
C3 -1.525845 0.440972 0.000188
N4 -0.425864 0.082503 0.000059
H5 1.046741 -0.421507 -0.000122
N6 2.980964 -0.047117 -0.000212
O7 1.956005 -0.932998 -0.000266
O8 4.090617 -0.543439 -0.000374
O9 2.715856 1.142527 -0.000011
B10 -3.009220 0.999147 0.000377
H11 -3.150505 1.678086 -0.992502
H12 -3.150383 1.677738 0.993511

F3.TS0
N1 -3.372154 -1.719660 -0.197094
C2 -2.843152 -0.783818 0.234903
C3 -0.870953 1.035703 -0.438733
N4 -1.555458 1.951262 -0.696865
H5 0.457008 0.026654 -0.407368
O6 1.220991 -0.687908 -0.494522
N7 2.363590 -0.197935 0.045197
O8 2.335601 0.910833 0.550726
O9 3.326809 -0.935498 -0.032930
B10 -2.184792 0.474646 0.892782
H11 -2.976230 1.323650 1.169168
H12 -1.391245 0.230069 1.752413

$O_3NH\cdot CNBH_2CN^-$
N1 4.845258 -1.046157 0.000374
C2 4.049160 -0.204070 0.000124
C3 0.466205 0.091710 -0.000237
N4 1.565843 0.457304 -0.000225
H5 -1.069037 -0.431920 -0.000235
O6 -2.005053 -0.942162 -0.000285
N7 -3.022657 -0.052962 0.000074
O8 -2.750648 1.137056 0.000394
O9 -4.137886 -0.538431 0.000040
B10 3.013846 1.001648 -0.000225
H11 3.168524 1.669636 0.996022
H12 3.168687 1.669205 -0.996735

$O_2NO^-\cdot HCN$
C1 2.361547 -0.093333 0.000049
N2 3.500978 0.083035 -0.000101
H3 1.269365 -0.285945 0.000164
O4 -0.397515 -0.886877 0.000090
N5 -1.301049 0.016894 0.000007
O6 -0.956140 1.221352 0.000049
O7 -2.501113 -0.316171 -0.000115

BH_2CN
N1 -1.343481 -0.000011 -0.000055
C2 -0.185556 0.000029 0.000106
B3 1.338858 -0.000007 -0.000026
H4 1.911748 1.036662 -0.000060
H5 1.911665 -1.036722 -0.000060

F3.TS1
C1 0.592630 -0.623557 -0.154858
N2 0.662202 0.514935 0.131296
B3 -1.012593 0.007765 -0.004662
H4 -1.546282 0.689555 -0.806085
H5 -1.581949 -0.591584 0.839476

$O_2NO^-\cdot HCN$
C1 2.361547 -0.093333 0.000049
N2 3.500978 0.083035 -0.000101
H3 1.269365 -0.285945 0.000164
O4 -0.397515 -0.886877 0.000090
N5 -1.301049 0.016894 0.000007
O6 -0.956140 1.221352 0.000049
O7 -2.501113 -0.316171 -0.000115

BH_2NC
B1 1.226055 0.000000 0.000008
H2 1.789443 -1.043358 0.000012
H3 1.789443 1.043358 0.000012
N4 -0.202215 0.000000 -0.000002
C5 -1.382277 0.000000 -0.000009

$BH_2(ONO_2)CN^-$
B1 0.886347 0.764545 0.000056
H2 0.767843 1.428360 -1.003076
H3 0.767876 1.428271 1.003254
O4 -0.144845 -0.402884 0.000033
N5 -1.441669 -0.095121 -0.000006
O6 -1.783231 1.080440 -0.000047
O7 -2.208949 -1.053933 0.000002
C8 2.293689 0.024890 -0.000001
N9 3.351186 -0.450261 -0.000045

HCN
C1 0.000000 0.000000 -0.498363
N2 0.000000 0.000000 0.650769
H3 0.000000 0.000000 -1.565209

Cartesian coordinates for the structures in Figure 3b, calculated at B3LYP/ 6-311++G(d,p)

$DCBH^-$
B1 0.000000 0.000000 0.916166
C2 0.000000 1.316283 0.026260
C3 0.000000 -1.316283 0.026260
N4 0.000000 2.304968 -0.580606
N5 0.000000 -2.304968 -0.580606
H6 0.992485 0.000000 1.616267
H7 -0.992485 0.000000 1.616267

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$O_3NH{\cdot}NCBH_2CN^-{\cdot}HNO_3$
C1 -1.303627 1.013566 0.022980
N2 -2.284749 0.402570 0.039911
C3 1.303620 1.013386 -0.021348
N4 2.284662 0.402270 -0.038610
H5 3.649791 -0.432184 -0.068845
N6 5.605634 -0.470861 0.007495
O7 4.416161 -1.120153 -0.110626
O8 6.584457 -1.186944 -0.028749
O9 5.587189 0.739901 0.135955
B10 0.000062 1.908702 0.001078
H11 -0.016643 2.596557 -0.992104
H12 0.016886 2.595942 0.994688
H13 -3.649875 -0.431883 0.070144
O14 -4.416247 -1.119815 0.112509
N15 -5.605622 -0.470894 -0.008566
O16 -5.587114 0.739571 -0.139802
O17 -6.584434 -1.186968 0.028128

F3.TS0'
N1 -1.491732 0.626849 0.024538
C2 -0.522721 1.181550 0.322210
C3 2.022109 1.578198 -0.569204
N4 1.898578 2.688103 -0.928621
H5 2.666183 -0.017004 -0.430442
O6 2.933803 -1.014350 -0.449514
N7 4.172692 -1.147691 0.103248
O8 4.719835 -0.147471 0.529667
O9 4.607496 -2.279566 0.109879
B10 0.750441 1.969626 0.791821
H11 0.506040 3.124798 0.962711
H12 1.320850 1.446614 1.701653
H13 -2.873012 -0.113895 -0.394254
O14 -3.659353 -0.616583 -0.818766
N15 -4.714345 -0.591586 0.042785
O16 -4.568803 -0.021318 1.108331
O17 -5.711096 -1.155318 -0.355903

$O_3NH{\cdot}CNBH_2CN^-{\cdot}HNO_3$
N1 -2.275530 0.410180 -0.040016
C2 -1.297687 1.026206 -0.024009
C3 2.240884 0.441232 0.036455
N4 1.261854 1.062622 0.018842
H5 3.663457 -0.447502 0.066175
O6 4.444365 -1.143605 0.104485
N7 5.633311 -0.496717 -0.005357
O8 5.617446 0.716461 -0.124286
O9 6.613382 -1.211964 0.027127
B10 0.000862 1.943101 -0.003401
H11 0.004880 2.622791 -1.000789
H12 -0.028236 2.625344 0.991808
H13 -3.634170 -0.438912 -0.068744
O14 -4.393255 -1.134271 -0.109466
N15 -5.588927 -0.496148 0.009342
O16 -5.581694 0.714783 0.136867
O17 -6.560792 -1.221581 -0.025453

$O_2NO^-{\cdot}HCN$
C1 2.361547 -0.093333 0.000049
N2 3.500978 0.083035 -0.000101
H3 1.269365 -0.285945 0.000164
O4 -0.397515 -0.886877 0.000090
N5 -1.301049 0.016894 0.000007
O6 -0.956140 1.221352 0.000049
O7 -2.501113 -0.316171 -0.000115

$BH_2CN{\cdot}HNO_3$
B1 4.228333 0.284791 0.000080
C2 2.749630 -0.112779 -0.000009
N3 1.632756 -0.405990 -0.000074
H4 -0.220847 -0.712413 -0.000082
O5 -1.159579 -1.018330 -0.000039
N6 -1.932423 0.139585 -0.000005
O7 -3.116740 -0.055602 0.000113
O8 -1.332295 1.194961 -0.000067
H9 4.774042 0.430920 -1.039170
H10 4.773944 0.430816 1.039395

$BH_2(\text{-}ONO_2)CN^-{\cdot}HNO_3$
B1 1.810268 0.934766 0.000047

H2 1.988590 1.580718 1.003320
H3 1.988576 1.580809 -1.003169
O4 4.624906 -1.265084 -0.000068
N5 3.993903 -0.216366 -0.000017
O6 2.660492 -0.354362 -0.000017
O7 4.476866 0.906360 0.000033
H8 -2.290852 -0.439142 0.000026
O9 -3.197428 -0.941643 0.000033
N10 -4.213755 -0.041674 -0.000011
O11 -3.932528 1.143571 -0.000049
O12 -5.327555 -0.525945 -0.000007
C13 0.316699 0.386619 0.000034
N14 -0.790986 0.055311 0.000028

HCN
C1 0.000000 0.000000 -0.498363
N2 0.000000 0.000000 0.650769
H3 0.000000 0.000000 -1.565209

F3.TS1'
N1 -1.165741 1.550845 0.015371
C2 -2.005888 0.734877 0.026319
C3 2.042530 0.111074 0.036225
N4 0.909309 -0.140811 0.031062
H5 3.713412 0.473464 0.046065
O6 4.676812 0.857423 0.066814
N7 5.565376 -0.169862 -0.022086
O8 5.123231 -1.302085 -0.106561
O9 6.732162 0.159473 -0.007303
B10 -0.521471 -0.600576 0.025117
H11 -0.824544 -1.124533 1.050991
H12 -0.818324 -1.122462 -1.003497
H13 -3.431330 -0.150263 0.049228
O14 -4.221961 -0.836236 0.084553
N15 -5.401185 -0.171432 -0.019882
O16 -6.391221 -0.873867 0.012270
O17 -5.369776 1.041516 -0.134135

$O_3NH \cdot CNBH_2NC^- \cdot HNO_3$
N1 1.249980 1.073118 0.046274
C2 2.224319 0.444123 0.044262
C3 -2.224292 0.444015 0.043991
N4 -1.249980 1.073051 0.046131
H5 -3.640044 -0.458012 0.043673
O6 -4.415161 -1.161079 0.058125
N7 -5.608990 -0.519837 -0.030851
O8 -5.602132 0.696712 -0.109294
O9 -6.583608 -1.243109 -0.022765
B10 -0.000024 1.974588 0.049338
H11 -0.000101 2.640486 1.053822
H12 0.000010 2.647924 -0.950045
H13 3.640070 -0.457902 0.044299
O14 4.415183 -1.160964 0.059239
N15 5.608989 -0.519848 -0.030912
O16 6.583597 -1.243128 -0.022356
O17 5.602125 0.696611 -0.110756

$O_2NO^- \cdot HCN$
N1 1.249980 1.073118 0.046274
C2 2.224319 0.444123 0.044262
C3 -2.224292 0.444015 0.043991
N4 -1.249980 1.073051 0.046131
H5 -3.640044 -0.458012 0.043673
O6 -4.415161 -1.161079 0.058125
N7 -5.608990 -0.519837 -0.030851
O8 -5.602132 0.696712 -0.109294
O9 -6.583608 -1.243109 -0.022765
B10 -0.000024 1.974588 0.049338
H11 -0.000101 2.640486 1.053822
H12 0.000010 2.647924 -0.950045
H13 3.640070 -0.457902 0.044299
O14 4.415183 -1.160964 0.059239
N15 5.608989 -0.519848 -0.030912
O16 6.583597 -1.243128 -0.022356
O17 5.602125 0.696611 -0.110756

$BH_2NC \cdot HNO_3$
N1 -2.788691 -0.114882 -0.000014
C2 -1.657138 -0.424665 -0.000036
B3 -4.168795 0.280290 0.000027
H4 -4.702119 0.431588 1.045937
H5 -4.702033 0.432280 -1.045825
H6 0.276272 -0.767204 -0.000043
O7 1.228510 -1.043906 -0.000036
N8 1.963515 0.137354 0.000006
O9 3.153421 -0.018228 0.000024
O10 1.329433 1.173706 0.000021

Cartesian coordinates for the structures in Figure 4a, calculated at B3LYP/ 6-311++G(d,p)

$DCBH^-$
B1 0.000000 0.000000 0.916166
C2 0.000000 1.316283 0.026260
C3 0.000000 -1.316283 0.026260
N4 0.000000 2.304968 -0.580606
N5 0.000000 -2.304968 -0.580606
H6 0.992485 0.000000 1.616267
H7 -0.992485 0.000000 1.616267

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$NCBH_2CN^-\cdot HNO_3$
C1 -4.067338 -0.179653 0.000235
N2 -4.875168 -1.010628 0.000139
C3 -1.525845 0.440972 0.000188
N4 -0.425864 0.082503 0.000059
H5 1.046741 -0.421507 -0.000122
N6 2.980964 -0.047117 -0.000212
O7 1.956005 -0.932998 -0.000266
O8 4.090617 -0.543439 -0.000374
O9 2.715856 1.142527 -0.000011
B10 -3.009220 0.999147 0.000377
H11 -3.150505 1.678086 -0.992502
H12 -3.150383 1.677738 0.993511

F4.TS0
C1 -2.649115 0.956627 -0.210290
N2 -3.545936 1.668377 -0.042601
N3 2.286725 0.199618 -0.023712
H4 0.069278 0.973097 1.198200
O5 2.072019 0.902439 1.002695
O6 1.303081 -0.316611 -0.630580
O7 3.444497 0.017487 -0.436985
H8 -0.679878 1.051553 1.320215
B9 -1.494139 -0.010712 -0.547075
H10 -0.828344 0.213270 -1.489309
C11 -1.543842 -1.410201 0.077631
N12 -1.667846 -2.480771 0.497911

$NCBH(-ONO_2)CN^-$
B1 0.732564 0.009347 0.446903
C2 1.967020 0.963838 0.139275
C3 1.009468 -1.460646 -0.100863
N4 2.879846 1.654848 -0.027619
N5 1.226894 -2.534784 -0.472131
H6 0.538122 -0.021931 1.632358
O7 -0.438472 0.669240 -0.297419
N8 -1.694306 0.267702 0.002645
O9 -2.577284 0.883444 -0.571855
O10 -1.852608 -0.647474 0.792072

H_2
H1 0.000000 0.000000 0.372217
H2 0.000000 0.000000 -0.372217

F4.TS1
N1 -2.407336 -0.145964 -0.025199
H2 -0.096755 -0.781209 1.336960
O3 -2.174012 -0.718070 1.075953
O4 -1.439488 0.305733 -0.701298
O5 -3.576317 -0.028915 -0.441918
H6 0.638265 -0.865650 1.510827
B7 1.597274 0.088841 -0.502766
H8 0.778996 -0.078786 -1.328338
N9 1.818715 1.386309 0.073002
N10 3.471137 -1.809558 -0.074368
C11 2.656154 -1.000305 -0.209165
C12 2.016186 2.466297 0.495571

$CNBH(-ONO_2)CN^-$
B1 -0.739182 0.057407 0.437750
C2 -1.991527 -0.886827 0.141860
N3 -2.912982 -1.570377 -0.005855
H4 -0.533640 0.103156 1.618710
O5 0.410344 -0.628680 -0.306225
N6 1.681520 -0.279106 0.006290
O7 2.540900 -0.913766 -0.582521
O8 1.873959 0.609385 0.816878
C9 -1.163012 2.531572 -0.530805
N10 -0.974944 1.450315 -0.128842

$CNBH\text{-}ONO_2$
B1 -0.910933 0.443294 0.256413
H2 -0.647662 1.451612 0.808043
O3 0.036216 -0.427900 -0.207695
N4 1.467004 -0.029761 -0.031295
O5 2.162752 -0.971948 0.161124
O6 1.702922 1.133720 -0.151155
N7 -2.267741 0.029518 0.045432
C8 -3.401272 -0.256225 -0.101209

CNBHO•
B1 0.609420 0.452965 0.000028
H2 0.948295 1.608959 -0.000890
O3 1.619570 -0.383646 -0.000122
N4 -0.775640 0.064833 0.000705
C5 -1.920412 -0.209742 -0.000535

CN^-
C1 0.000000 0.000000 -0.632839
N2 0.000000 0.000000 0.542434

Cartesian coordinates for the structures in Figure 4b, calculated at B3LYP/ 6-311++G(d,p)

$DCBH^-$
B1 0.000000 0.000000 0.916166
C2 0.000000 1.316283 0.026260
C3 0.000000 -1.316283 0.026260
N4 0.000000 2.304968 -0.580606
N5 0.000000 -2.304968 -0.580606
H6 0.992485 0.000000 1.616267
H7 -0.992485 0.000000 1.616267

HNO_3
N1 -0.153280 0.030474 -0.000015
O2 -0.233041 1.237718 0.000001
O3 -1.009422 -0.801601 -0.000167
O4 1.160919 -0.499325 0.000158
H5 1.725304 0.292345 0.000173

$O_3NH \cdot NCBH_2CN^- \cdot HNO_3$
C1 -1.303627 1.013566 0.022980
N2 -2.284749 0.402570 0.039911
C3 1.303620 1.013386 -0.021348
N4 2.284662 0.402270 -0.038610
H5 3.649791 -0.432184 -0.068845
N6 5.605634 -0.470861 0.007495
O7 4.416161 -1.120153 -0.110626
O8 6.584457 -1.186944 -0.028749
O9 5.587189 0.739901 0.135955
B10 0.000062 1.908702 0.001078
H11 -0.016643 2.596557 -0.992104
H12 0.016886 2.595942 0.994688
H13 -3.649875 -0.431883 0.070144
O14 -4.416247 -1.119815 0.112509
N15 -5.605622 -0.470894 -0.008566
O16 -5.587114 0.739571 -0.139802
O17 -6.584434 -1.186968 0.028128

F4.TS0'
C1 1.570037 3.048025 0.005799
N2 1.614824 4.151650 0.350286
N3 3.169577 -1.603257 -0.045070
H4 2.881414 0.616101 1.218172
O5 3.456870 -1.238422 1.127190
O6 2.452406 -0.839660 -0.764486
O7 3.576484 -2.680463 -0.497161
H8 2.694519 1.356992 1.269724
B9 1.488280 1.616387 -0.565629
H10 2.108534 1.364846 -1.531541
C11 0.236496 0.797522 -0.195691
N12 -0.762579 0.273122 0.043767
H13 -2.283433 -0.465358 0.367563
O14 -3.095265 -0.971692 0.678718
N15 -4.178777 -0.474733 -0.000641
O16 -3.981059 0.417961 -0.801826
O17 -5.232305 -0.994634 0.283213

$NCBH(-ONO_2)CN^- \cdot HNO_3$
N1 -2.461818 3.381619 -0.273285
C2 -2.216618 2.286364 0.004803
H3 2.304969 -0.136985 -0.496542
O4 3.201448 -0.431190 -0.889706
N5 4.185837 -0.165243 0.016300
O6 3.866064 0.348307 1.071721
O7 5.301608 -0.477930 -0.339710
B8 -1.876041 0.803988 0.455100
H9 -2.024549 0.688788 1.640777
O10 -2.842917 -0.071546 -0.335545
N11 -2.958431 -1.375782 0.029152
O12 -3.829476 -1.990709 -0.556367
O13 -2.202897 -1.816441 0.877346
C14 -0.357662 0.459329 0.089671
N15 0.747959 0.226572 -0.144807

F4.TS1′
C1 1.471430 3.039658 -0.035140
N2 1.533763 4.160670 0.241363
N3 3.369602 -1.576043 -0.044948
H4 2.995576 0.726860 1.190899
O5 4.090834 -0.904814 0.744998
O6 2.279538 -1.074858 -0.451948
O7 3.718662 -2.707223 -0.418561
H8 2.620401 1.356254 1.404355
B9 1.372525 1.575078 -0.522224
H10 2.070250 1.186284 -1.382282
H11 -2.434700 -0.511614 0.421432
O12 -3.256878 -1.015557 0.721730
N13 -4.321962 -0.527507 0.005241
O14 -4.099654 0.355276 -0.801404
O15 -5.382676 -1.042745 0.265451
C16 -0.827595 0.300003 0.076863
N17 0.164914 0.864054 -0.166763

$NCBH(-ONO_2)NC^- \cdot HNO_3$
N1 -2.446183 3.374008 -0.288949
C2 -2.196540 2.280077 -0.010504
C3 0.707851 0.210959 -0.132619
N4 -0.400272 0.463367 0.101101
H5 2.340504 -0.177180 -0.496720

O6 3.252945 -0.485404 -0.877823
N7 4.235990 -0.168249 0.009948
O8 3.914961 0.396788 1.039799
O9 5.354565 -0.490471 -0.329567
B10 -1.859142 0.796611 0.453338
H11 -2.027115 0.673470 1.632421
O12 -2.796843 -0.076195 -0.360830
N13 -2.970118 -1.370150 0.030481
O14 -3.816312 -1.976525 -0.598102
O15 -2.286999 -1.807993 0.937559

Cartesian coordinates for the structures in Figure 4c, calculated at B3LYP/ 6-311++G(d,p)

F4.TS0''

C1 -1.488442 0.625961 -0.166948
N2 -2.535326 0.242059 0.130612
N3 2.125919 3.775887 0.010115
H4 0.161898 2.712491 1.118165
O5 1.649030 3.823543 1.177288
O6 1.683909 2.891547 -0.792623
O7 2.997677 4.564744 -0.357855
H8 -0.470749 2.274387 1.067108
B9 -0.105786 1.110331 -0.685858
H10 -0.111182 1.720870 -1.690003
C11 1.101265 0.249649 -0.272514
N12 1.953212 -0.476439 0.005539
H13 3.218386 -1.610685 0.374506
O14 3.985045 -2.164382 0.709873
N15 3.966400 -3.351610 0.017687
O16 3.093766 -3.502970 -0.814598
O17 4.840912 -4.125698 0.325232
H18 -4.133614 -0.332526 0.563451
O19 -4.984359 -0.636774 0.995150
N20 -5.868059 -0.945963 -0.015105
O21 -5.481904 -0.805433 -1.158160
O22 -6.947550 -1.329249 0.364555

$O_3NH \cdot NCBH(-ONO_2)CN^- \cdot HNO_3$

H1 -3.584520 -0.961502 -0.445648
O2 -4.439960 -1.358824 -0.821655
N3 -4.865855 -2.343751 0.026831
O4 -4.197436 -2.566705 1.017775
O5 -5.887173 -2.897328 -0.313623
B6 0.068038 1.339669 0.492279
H7 0.090691 1.555396 1.671869
O8 0.179059 2.599439 -0.344303
N9 -0.649049 3.638108 -0.026140
O10 -0.440499 4.656908 -0.651379
O11 -1.503720 3.459525 0.821567
H12 3.686970 -0.988893 -0.498283
O13 4.437916 -1.544365 -0.894681
N14 5.435561 -1.643940 0.036707
O15 6.398109 -2.284771 -0.320533
O16 5.267420 -1.094361 1.108311
C17 1.360176 0.498561 0.097132
C18 -1.243247 0.503355 0.133823
N19 2.305747 -0.118619 -0.137183
N20 -2.189922 -0.113368 -0.098343

Cartesian coordinates for the condensed-phase structures in Figure 6a, calculated at SMD-GIL//B3LYP/6-311++G(d,p)

DCA^-
N1 0.000000 2.238858 -0.378443
C2 0.000000 1.151474 0.056566
N3 0.000000 0.000000 0.659917
C4 0.000000 -1.151474 0.056566
N5 0.000000 -2.238858 -0.378443

HNO_3
N1 -0.139224 0.028370 -0.000016
O2 -0.989101 -0.821616 -0.000137
O3 1.158883 -0.474070 0.000126
O4 -0.265782 1.232045 -0.000003
H5 1.742575 0.310537 0.000219

$O_3NH{\cdot}NCNCN^-{\cdot}HNO_3$
N1 -5.599492 -0.183196 -0.003264
O2 -6.696912 -0.700288 0.033025
O3 -4.557268 -1.047315 -0.004220
O4 -5.357084 1.010445 -0.037774
H5 -3.671129 -0.506922 -0.028532
N6 -0.000098 1.092137 0.107388
C7 1.151358 0.517835 0.017661
N8 2.241810 0.108255 -0.049405
C9 -1.151434 0.517767 0.016579
N10 -2.241796 0.108120 -0.051559
H11 3.671136 -0.506841 -0.027595
O12 4.557273 -1.047285 -0.004398
N13 5.599528 -0.183202 -0.003417
O14 6.696961 -0.700371 0.031326
O15 5.357127 1.010484 -0.036398

F1.TS0′
N1 -3.094391 1.234997 0.117431
O2 -2.840414 2.392751 -0.173478
O3 -4.209333 0.821790 0.432284
O4 -2.065271 0.391873 0.100389
H5 -4.158542 -1.171601 0.101412
N6 -1.037670 -1.791288 -0.129864
C7 0.059820 -1.134744 -0.271909
N8 1.120369 -0.664685 -0.395918
C9 -2.256994 -1.358673 -0.061292
N10 -3.400297 -1.824681 -0.077171
H11 2.509780 0.022018 -0.551748
O12 3.377836 0.541896 -0.782430
N13 4.321749 0.258614 0.145681
O14 5.387655 0.815716 -0.017764
O15 4.032465 -0.511603 1.044552

$HNC(\text{-}ONO_2)NCN^-{\cdot}HNO_3$
N1 -1.203066 -1.665646 0.092277
C2 -2.411180 -1.150373 -0.183171
N3 -3.571176 -1.657281 -0.104308
C4 -0.098929 -1.016520 -0.030685
N5 0.964286 -0.532698 -0.106251
H6 -3.510544 -2.607212 0.261380
O7 -2.375750 0.192120 -0.745623
N8 -2.837470 1.223824 0.103457
O9 -3.041224 0.964483 1.261305
O10 -2.948632 2.276687 -0.469825
H11 2.274614 0.222344 -0.105129
O12 3.100604 0.873768 -0.125921
N13 4.236716 0.165205 0.035928
O14 5.262118 0.817486 0.022561
O15 4.149329 -1.042994 0.179898

F1.TS3′
N1 0.925195 1.732283 0.337054
C2 1.916008 0.830722 0.143328
N3 3.164309 1.000590 0.502509
C4 -0.278193 1.481110 -0.049481
N5 -1.401247 1.380352 -0.366484
H6 3.409975 1.734687 1.161294
O7 1.695653 -0.319135 -0.449716
N8 3.398994 -0.937893 -0.092000
O9 3.348761 -1.656541 0.852113
O10 4.042115 -0.938237 -1.088136
H11 -2.717800 0.722315 -0.588758
O12 -3.624492 0.261583 -0.890063
N13 -4.073770 -0.527820 0.104481
O14 -4.996018 -1.263874 -0.190678
O15 -3.542697 -0.441367 1.199662

$O_2N\text{-}NHC(O)NCN^-{\cdot}HNO_3$
N1 0.838378 -0.598299 -0.200657
C2 1.875579 0.264968 -0.106847
N3 3.078975 -0.551463 -0.269563
C4 -0.378858 -0.158891 -0.122664
N5 -1.512151 0.115964 -0.067251
O6 1.926242 1.461841 0.064567
H7 2.954316 -1.544135 -0.121664
N8 4.360207 -0.171728 0.054399
O9 5.118110 -1.104214 0.352008
O10 4.675405 0.999782 -0.017444
H11 -2.989367 0.463077 0.003506
O12 -3.958253 0.871182 0.055143
N13 -4.879822 -0.116217 0.053902

O14 -6.037389 0.255148 0.111035
O15 -4.492163 -1.271639 -0.002882

O_2N-NHC(O)NCNH·NO_3^-
N1 -0.849837 2.028517 -0.436819
C2 -1.796193 1.020678 -0.320712
N3 -1.211640 -0.216086 0.048074
C4 0.224575 2.081576 0.184043
N5 1.235437 2.260290 0.797605
O6 -2.967092 1.178869 -0.554837
H7 -0.212290 -0.397126 -0.111417
N8 -1.918582 -1.388350 0.254364
O9 -1.239591 -2.408992 0.221332
O10 -3.110754 -1.332427 0.488439
H11 2.080696 1.644898 0.659798
O12 3.474109 -1.593079 -0.322529
N13 2.752674 -0.597151 -0.182164
O14 3.195071 0.419075 0.440193
O15 1.586373 -0.572425 -0.659571

F1.TS3c'
C1 -1.266752 1.205862 -0.224392
N2 -1.264651 -0.173020 0.190250
C3 1.081316 1.364329 0.251037
N4 2.120384 1.623642 0.879221
O5 -2.282004 1.759718 -0.598901
H6 -0.404479 -0.699950 0.035516
N7 -2.367261 -0.996306 0.135717
O8 -2.123009 -2.192459 -0.028125
O9 -3.476910 -0.522625 0.303105
H10 2.040443 2.463220 1.451068
O11 3.398676 -0.871083 -0.916710
N12 2.420076 -0.848607 -0.188332
O13 2.320155 -1.423790 0.883946
O14 1.356353 -0.139941 -0.620041
N15 -0.061324 1.813866 -0.135805

O_2N-NHC(O)NC(-ONO_2)NH^-
N1 -0.131960 1.292521 -0.062156
C2 0.613525 0.178528 -0.129293
N3 2.000151 0.615565 -0.107409
C4 -1.463451 1.304148 -0.196127
N5 -2.297733 2.251497 -0.029879
O6 0.327125 -1.007977 -0.179816
H7 2.185570 1.574014 0.167125
N8 3.103516 -0.171726 0.021562
O9 4.131135 0.412020 0.387531
O10 3.042571 -1.359276 -0.257950
H11 -1.799575 3.086497 0.279461
O12 -2.104407 0.109651 -0.754612
N13 -2.396121 -0.892731 0.169314
O14 -2.797935 -1.908109 -0.342849
O15 -2.252416 -0.649116 1.343434

F1.TS3d'
N1 -0.090852 0.802355 0.312519
C2 -1.038156 -0.142092 0.176070
N3 -2.310278 0.568607 0.137715
C4 1.213058 0.467955 0.241636
N5 2.190850 1.308519 0.510411
O6 -0.997629 -1.358266 0.103899
H7 -2.289344 1.560802 -0.069103
N8 -3.537499 0.030057 -0.092512
O9 -4.404872 0.827491 -0.471763
O10 -3.732142 -1.158130 0.117198
H11 1.999852 2.307629 0.524885
O12 1.665152 -0.716742 -0.113815
N13 3.386420 -0.156792 -0.188384
O14 4.003713 -0.610082 0.724984
O15 3.686976 0.054125 -1.325535

DNB^-
N1 0.000000 0.252813 0.000000
C2 1.167174 -0.423054 0.002070
O3 1.444957 -1.600808 -0.122766
N4 2.207458 0.582342 0.181628
N5 3.549378 0.411371 0.021579
O6 4.198226 1.450690 -0.148551
O7 4.035790 -0.706972 0.089968
C8 -1.167174 -0.423054 -0.002070
O9 -1.444957 -1.600808 0.122767
N10 -2.207458 0.582342 -0.181628
N11 -3.549378 0.411371 -0.021579
O12 -4.198226 1.450690 0.148551
O13 -4.035790 -0.706972 -0.089968
H14 -1.939032 1.554208 -0.075506
H15 1.939032 1.554208 0.075506

Cartesian coordinates for the condensed-phase structures in Figure 6b1, calculated at SMD-GIL//B3LYP/6-311++G(d,p)

$DCBH^-$
B1 0.000000 0.000000 0.930799
C2 0.000000 1.302662 0.031591
C3 0.000000 -1.302662 0.031591
N4 0.000000 2.279790 -0.591338
N5 0.000000 -2.279790 -0.591338
H6 0.992544 0.000000 1.622820
H7 -0.992544 0.000000 1.622820

HNO_3
N1 -0.139224 0.028370 -0.000016
O2 -0.989101 -0.821616 -0.000137
O3 1.158883 -0.474070 0.000126
O4 -0.265782 1.232045 -0.000003
H5 1.742575 0.310537 0.000219

$O_3NH \cdot NCBH_2CN^- \cdot HNO_3$
C1 -1.295876 1.026620 0.082681
N2 -2.269660 0.404705 0.098320
C3 1.295927 1.026388 0.083025
N4 2.269587 0.404287 0.098949
H5 3.615103 -0.474199 0.094252
N6 5.554383 -0.473487 -0.056431
O7 4.387897 -1.150889 0.104890
O8 6.549665 -1.164984 -0.066557
O9 5.501450 0.737010 -0.173975
B10 0.000108 1.927379 0.061043
H11 0.000296 2.587351 -0.949219
H12 0.000047 2.634992 1.038608
H13 -3.615111 -0.473955 0.093893
O14 -4.387777 -1.150781 0.104581
N15 -5.554413 -0.473542 -0.056338
O16 -5.501742 0.737031 -0.173216
O17 -6.549548 -1.165245 -0.066784

F2.TS0'
N1 2.189230 -1.393270 -0.089146
O2 2.441757 -2.548163 -0.445707
O3 1.309166 -1.110470 0.732536
O4 2.876348 -0.434987 -0.634817
H5 3.787766 2.012283 1.760938
C6 0.341770 1.176688 -0.513828
N7 -0.665445 0.622562 -0.402865
C8 2.773934 1.289196 0.272729
N9 3.598131 1.227074 1.138917
B10 1.693628 1.977609 -0.652431
H11 2.080036 1.953030 -1.792595
H12 1.546860 3.107481 -0.250878
H13 -2.039106 -0.143431 -0.054988
O14 -2.828320 -0.746423 0.204023
N15 -3.972774 -0.023926 0.098714
O16 -3.882590 1.148255 -0.218723
O17 -4.989100 -0.638185 0.341055

$HNC(-ONO_2)BH_2CN^- \cdot HNO_3$
B1 1.080727 1.905137 -0.468493
C2 -0.249505 1.085477 -0.240713
C3 2.357694 1.161118 0.174915
N4 -1.244260 0.517609 -0.079533
N5 3.226213 1.604846 0.957295
H6 1.253801 2.008037 -1.663455
H7 0.955958 2.987707 0.048695
H8 -2.591723 -0.266856 0.202678
O9 -3.382927 -0.886438 0.441533
N10 -4.536329 -0.287980 0.053375
O11 -5.543575 -0.930126 0.263375
O12 -4.466286 0.814654 -0.459013
O13 2.346143 -0.238508 -0.364511
H14 4.003584 0.982679 1.173762
N15 3.404573 -1.128211 -0.156180
O16 3.066342 -2.286422 -0.130872
O17 4.527082 -0.680744 -0.056654

F2.TS3'
C1 -2.210394 0.828236 0.086010
N2 -3.350076 0.946202 0.681343
C3 0.382373 1.404315 0.045583
N4 1.458996 0.983637 0.080253
H5 -3.592218 1.763569 1.235650
O6 -2.025758 -0.268896 -0.549890
N7 -3.784401 -0.961276 -0.098955
O8 -4.509635 -0.866332 -1.039671
O9 -3.702820 -1.781985 0.760759
B10 -1.069362 2.015450 0.034472
H11 -1.236825 2.601671 -1.009908
H12 -1.202692 2.746932 0.984331
H13 2.815913 0.207897 0.394082
O14 3.555642 -0.392436 0.789399
N15 4.603475 -0.459147 -0.066857
O16 4.559630 0.210491 -1.083204
O17 5.502292 -1.195657 0.280537

$O_2N\text{-}NHC(O)BH_2CN^- \cdot HNO_3$
C1 -1.430510 1.250617 -0.167607
N2 -1.394344 -0.192587 -0.044259
C3 1.289325 1.171288 0.049896

N4 2.117240 1.475644 0.953760
O5 -2.477052 1.848804 -0.023286
H6 -0.598494 -0.680504 -0.446471
N7 -2.479651 -1.035193 0.045003
O8 -2.320755 -2.169988 -0.412139
O9 -3.499207 -0.633274 0.581411
H10 1.870425 2.376314 1.359970
O11 3.671193 -0.682899 -0.589746
N12 2.614735 -0.854611 -0.052265
O13 2.314349 -1.603893 0.834035
O14 1.504173 -0.076901 -0.610081
B15 -0.003533 1.922299 -0.565441
H16 -0.007297 3.060182 -0.157716
H17 0.052681 1.893511 -1.779543

F2.TS3a'
C1 1.957240 0.716507 0.641779
N2 2.596121 0.399572 -0.407321
C3 -0.518155 1.061757 -0.402421
N4 -1.503110 0.457373 -0.409708
H5 3.069657 1.103437 -0.967112
O6 1.715407 0.487136 1.784127
N7 4.456465 -0.726727 -0.196898
O8 4.521430 -1.788712 0.416459
O9 5.419050 -0.266337 -0.813509
B10 0.792195 1.896802 -0.409954
H11 0.869561 2.742316 0.430259
H12 1.166968 2.188968 -1.500305
H13 -2.897366 -0.421227 -0.391280
O14 -3.677889 -1.073995 -0.424016
N15 -4.795583 -0.415351 -0.007335
O16 -5.803844 -1.085204 0.008268
O17 -4.684349 0.755717 0.302531

$OCNBH_2CN^{-}\cdot HNO_3$
C1 -4.257901 -0.477597 0.064145
N2 -3.366180 0.284368 -0.030731
C3 -0.871072 0.807251 -0.134656
N4 0.220097 0.401590 -0.215842
O5 -5.154574 -1.265450 0.146507
B6 -2.344331 1.413314 -0.029033
H7 -2.497065 2.144641 -0.983674
H8 -2.395385 2.051134 1.000541
H9 1.639627 -0.329726 -0.186505
O10 2.464788 -0.946534 -0.199943
N11 3.569819 -0.200977 0.055322
O12 4.614694 -0.816064 0.050303
O13 3.422863 0.989873 0.262710

HONO
H1 1.728448 0.421332 0.000052
N2 -0.161646 0.483876 0.000014
O3 -1.102918 -0.219095 -0.000033
O4 1.028302 -0.256963 0.000014

F2.TS3c'
C1 -1.448949 1.260415 -0.203138
N2 -1.311292 -0.141127 0.062594
C3 1.240330 1.455940 0.250531
N4 2.148525 1.551009 1.038022
O5 -2.544056 1.781063 -0.284184
H6 -0.414627 -0.577796 -0.163930
N7 -2.330732 -1.067161 0.111703
O8 -2.013051 -2.227848 -0.152891
O9 -3.449853 -0.703452 0.434517
H10 2.204145 2.362629 1.651095
O11 3.570336 -0.596314 -0.537827
N12 2.433579 -0.896802 -0.196192
O13 2.154033 -1.831449 0.550093
O14 1.431983 -0.149744 -0.652819
B15 -0.056420 2.063443 -0.435276
H16 -0.163749 3.160018 0.063550
H17 0.132349 2.140335 -1.626688

$O_2N\text{-}NHC(O)BH_2C(\text{-}ONO_2)NH^{-}$
C1 -1.430510 1.250617 -0.167607
N2 -1.394344 -0.192587 -0.044259
C3 1.289325 1.171288 0.049896
N4 2.117240 1.475644 0.953760
O5 -2.477052 1.848804 -0.023286
H6 -0.598494 -0.680504 -0.446471
N7 -2.479651 -1.035193 0.045003
O8 -2.320755 -2.169988 -0.412139
O9 -3.499207 -0.633274 0.581411
H10 1.870425 2.376314 1.359970
O11 3.671193 -0.682899 -0.589746
N12 2.614735 -0.854611 -0.052265
O13 2.314349 -1.603893 0.834035
O14 1.504173 -0.076901 -0.610081
B15 -0.003533 1.922299 -0.565441
H16 -0.007297 3.060182 -0.157716
H17 0.052681 1.893511 -1.779543

F2.TS3d'
C1 -1.545057 1.223753 -0.002805
N2 -1.635948 -0.173667 -0.349368
C3 1.204521 0.949666 -0.101518
N4 2.322242 1.370009 0.382330
O5 -2.505761 1.812242 0.454203

H6 -0.756541 -0.678302 -0.467202
N7 -2.666820 -1.031428 -0.053619
O8 -2.367239 -2.226347 0.024563
O9 -3.794585 -0.584433 0.085956
H10 2.437056 2.333529 0.686087
O11 1.168969 -0.292961 -0.436094
N12 3.006354 -0.655107 0.087458
O13 3.031858 -1.229648 1.128837
O14 3.704440 -0.710280 -0.874106
B15 -0.117195 1.907519 -0.365188
H16 -0.125184 2.117450 -1.562545
H17 -0.008383 2.931979 0.261057

O_2N-NHC(O)BH_2C(O)NH-NO_2^-
C1 -1.485962 1.185151 -0.020978
N2 -1.891466 -0.169046 0.253208
C3 1.044597 0.165687 0.102051
H4 -1.141636 -0.870098 0.268130
O5 -2.289828 2.017166 -0.396765
N6 -3.124233 -0.725898 0.027943
O7 -4.114641 -0.010089 0.039844
O8 -3.141676 -1.948174 -0.145331
B9 0.081103 1.453489 0.290239
H10 0.471484 2.389933 -0.368043
H11 0.148340 1.736348 1.474437
N12 2.402693 0.557734 -0.096687
N13 3.532206 -0.231289 -0.076987
O14 3.420469 -1.437943 -0.206841
O15 4.597400 0.373871 0.054727
O16 0.739722 -1.018601 0.147494
H17 2.638528 1.540994 -0.009511

Cartesian coordinates for the condensed-phase structures in Figure 6b2, calculated at SMD-GIL//B3LYP/6-311++G(d,p)

$DCBH^-$
B1 0.000000 0.000000 0.930799
C2 0.000000 1.302662 0.031591
C3 0.000000 -1.302662 0.031591
N4 0.000000 2.279790 -0.591338
N5 0.000000 -2.279790 -0.591338
H6 0.992544 0.000000 1.622820
H7 -0.992544 0.000000 1.622820

HNO_3
N1 -0.139224 0.028370 -0.000016
O2 -0.989101 -0.821616 -0.000137
O3 1.158883 -0.474070 0.000126
O4 -0.265782 1.232045 -0.000003
H5 1.742575 0.310537 0.000219

$O_3NH{\cdot}NCBH_2CN^-{\cdot}HNO_3$
C1 -1.295876 1.026620 0.082681
N2 -2.269660 0.404705 0.098320
C3 1.295927 1.026388 0.083025
N4 2.269587 0.404287 0.098949
H5 3.615103 -0.474199 0.094252
N6 5.554383 -0.473487 -0.056431
O7 4.387897 -1.150889 0.104890
O8 6.549665 -1.164984 -0.066557
O9 5.501450 0.737010 -0.173975
B10 0.000108 1.927379 0.061043
H11 0.000296 2.587351 -0.949219
H12 0.000047 2.634992 1.038608
H13 -3.615111 -0.473955 0.093893
O14 -4.387777 -1.150781 0.104581
N15 -5.554413 -0.473542 -0.056338
O16 -5.501742 0.737031 -0.173216
O17 -6.549548 -1.165245 -0.066784

F3.TS0′
C1 0.447784 1.516303 0.323956
N2 1.386254 0.952629 -0.043977
C3 -2.155498 1.705194 -0.346452
N4 -2.193509 2.806589 -0.746196
H5 -2.430498 0.025099 -0.059785
N6 -3.749685 -1.403439 0.029943
O7 -2.457290 -0.987971 0.125630
O8 -3.917251 -2.589996 0.207230
O9 -4.601331 -0.570019 -0.217852
B10 -0.790301 2.306521 0.866475
H11 -1.257037 1.846105 1.861708
H12 -0.592935 3.481004 0.892719
H13 2.728306 0.149375 -0.535291
O14 3.508678 -0.338734 -0.975159
N15 4.414354 -0.648458 -0.006812
O16 4.159925 -0.322492 1.137418
O17 5.400775 -1.230090 -0.400699

$O_3NH{\cdot}CNBH_2CN^-{\cdot}HNO_3$
N1 2.265293 0.409324 0.070076
C2 1.285693 1.019829 0.020506
C3 -2.222731 0.362338 -0.074753
N4 -1.261063 1.009010 -0.059018
H5 -3.631384 -0.523824 -0.105767
O6 -4.447531 -1.179073 -0.155810
N7 -5.588282 -0.472083 0.023162
O8 -5.496581 0.727947 0.218023
O9 -6.611937 -1.121578 -0.029213
B10 -0.021658 1.916400 -0.044403
H11 -0.050866 2.621752 0.932986
H12 0.009748 2.568686 -1.057888
H13 3.611760 -0.475699 0.098542
O14 4.380909 -1.154448 0.127653
N15 5.552868 -0.478751 -0.001492
O16 5.504742 0.731985 -0.117378
O17 6.546592 -1.172135 0.013040

F3.TS1′
N1 -2.897091 -2.442795 -0.907756
C2 -2.911134 -1.398543 -0.373409
C3 0.601199 -1.116590 -0.008515
N4 -0.344900 -1.712414 0.303216
H5 1.975973 -0.182870 -0.407207
O6 2.711175 0.514298 -0.622367
N7 3.856031 0.136750 -0.001144
O8 3.885545 -0.959022 0.531376
O9 4.758525 0.944878 -0.053606
B10 -1.590894 -2.408442 0.739717
H11 -2.034556 -1.998067 1.763668
H12 -1.576330 -3.586630 0.590783
H13 -3.040910 0.152247 0.225549
O14 -3.116464 1.113879 0.629719
N15 -2.164372 1.869523 0.024491
O16 -2.133704 3.034327 0.363724
O17 -1.437298 1.325500 -0.787779

$O_3NH{\cdot}CNBH_2NC^-{\cdot}HNO_3$
C1 2.218054 0.326822 0.048866
N2 1.245919 0.957645 0.024783
H3 3.645823 -0.538743 0.103369

O4 4.471842 -1.177076 0.173828
N5 5.600902 -0.452415 -0.012292
O6 5.487824 0.740589 -0.235996
O7 6.635924 -1.080960 0.064018
B8 -0.000008 1.860517 0.000034
H9 0.019067 2.529629 -1.000834
H10 -0.019092 2.529589 1.000928
H11 -3.645821 -0.538770 -0.103364
O12 -4.471847 -1.177096 -0.173803
N13 -5.600899 -0.452412 0.012273
O14 -5.487808 0.740604 0.235909
O15 -6.635928 -1.080949 -0.064005
C16 -2.218049 0.326793 -0.048861
N17 -1.245924 0.957630 -0.024751

$BH_2CN \cdot HNO_3$
B1 4.207227 0.237842 0.019353
C2 2.702141 -0.092596 -0.010151
N3 1.566716 -0.335968 -0.032735
H4 -0.150614 -0.673481 -0.029346
O5 -1.100234 -0.992867 -0.038025
N6 -1.898708 0.121912 0.007910
O7 -3.083700 -0.108992 0.001360
O8 -1.350202 1.204902 0.050137
H9 4.846980 -0.165794 0.926456
H10 4.651678 0.879693 -0.866980

$O_2NO^- \cdot HCN$
C1 2.395377 -0.137728 -0.000020
N2 3.516502 0.120739 -0.000370
H3 1.329926 -0.386507 0.000298
O4 -0.467343 -0.932716 0.000592
N5 -1.307103 0.017342 0.000077
O6 -0.898175 1.202131 0.000359
O7 -2.530480 -0.238627 -0.000717

$BH_2(\text{-}ONO_2)CN^- \cdot HNO_3$
B1 -1.816587 0.964647 -0.000668
C2 -0.320954 0.437791 0.042293
N3 0.783908 0.101137 0.065232
H4 -2.032671 1.635827 0.976182
H5 -1.993302 1.566239 -1.029240
H6 2.298147 -0.460919 0.029354
O7 3.191114 -0.963706 -0.006554
N8 4.198331 -0.051127 -0.012053
O9 5.313630 -0.522096 -0.063866
O10 3.901565 1.128353 0.034221
O11 -2.640002 -0.344360 0.028906
N12 -3.971258 -0.232868 -0.012059
O13 -4.474250 0.879060 -0.074009
O14 -4.584605 -1.291141 0.016982
$O_3NH \cdot CNBH_2NC^- \cdot HNO_3$

HCN
C1 0.000000 0.000000 -0.497769
N2 0.000000 0.000000 0.650954
H3 0.000000 0.000000 -1.570062

Cartesian coordinates for the condensed-phase structures in Figure 6b3, calculated at SMD-GIL//B3LYP/6-311++G(d,p)

$DCBH^-$
B1 0.000000 0.000000 0.930799
C2 0.000000 1.302662 0.031591
C3 0.000000 -1.302662 0.031591
N4 0.000000 2.279790 -0.591338
N5 0.000000 -2.279790 -0.591338
H6 0.992544 0.000000 1.622820
H7 -0.992544 0.000000 1.622820

HNO_3
N1 -0.139224 0.028370 -0.000016
O2 -0.989101 -0.821616 -0.000137
O3 1.158883 -0.474070 0.000126
O4 -0.265782 1.232045 -0.000003
H5 1.742575 0.310537 0.000219

$O_3NH{\cdot}NCBH_2CN^-{\cdot}HNO_3$
C1 -1.295876 1.026620 0.082681
N2 -2.269660 0.404705 0.098320
C3 1.295927 1.026388 0.083025
N4 2.269587 0.404287 0.098949
H5 3.615103 -0.474199 0.094252
N6 5.554383 -0.473487 -0.056431
O7 4.387897 -1.150889 0.104890
O8 6.549665 -1.164984 -0.066557
O9 5.501450 0.737010 -0.173975
B10 0.000108 1.927379 0.061043
H11 0.000296 2.587351 -0.949219
H12 0.000047 2.634992 1.038608
H13 -3.615111 -0.473955 0.093893
O14 -4.387777 -1.150781 0.104581
N15 -5.554413 -0.473542 -0.056338
O16 -5.501742 0.737031 -0.173216
O17 -6.549548 -1.165245 -0.066784

F4.TS0′
C1 1.57004 3.04802 0.0058
N2 1.61482 4.15165 0.35029
N3 3.16958 -1.60326 -0.04507
H4 2.88141 0.6161 1.21817
O5 3.45687 -1.23842 1.12719
O6 2.45241 -0.83966 -0.76449
O7 3.57648 -2.68046 -0.49716
H8 2.69452 1.35699 1.26972
B9 1.48828 1.61639 -0.56563
H10 2.10853 1.36485 -1.53154
C11 0.2365 0.79752 -0.19569
N12 -0.76258 0.27312 0.04377
H13 -2.28343 -0.46536 0.36756
O14 -3.09526 -0.97169 0.67872
N15 -4.17878 -0.47473 -0.00064
O16 -3.98106 0.41796 -0.80183
O17 -5.23231 -0.99463 0.28321

$NCBH(ONO_2)CN^-{\cdot}HNO_3$
N1 -2.459419 3.372545 -0.284231
C2 -2.209444 2.282727 0.007426
H3 2.298593 -0.182539 -0.561582
O4 3.208219 -0.476540 -0.910896
N5 4.143297 -0.151818 0.026050
O6 3.762695 0.389916 1.046394
O7 5.280247 -0.446175 -0.267838
B8 -1.861792 0.805175 0.464915
H9 -1.987728 0.701729 1.652199
O10 -2.851390 -0.066917 -0.301474
N11 -2.918489 -1.377189 0.038199
O12 -3.795271 -2.004352 -0.524752
O13 -2.117878 -1.814687 0.845432
C14 -0.359608 0.453892 0.062220
N15 0.737388 0.211499 -0.198304

H_2
H1 0.000000 0.000000 0.372435
H2 0.000000 0.000000 -0.372435