

ELECTRONIC SUPPORTING INFORMATION

Uptake and reactions of dimethylamine on hydrated nitric-acid clusters: mimicking atmospheric clusters in molecular-beam experiments

Andriy Pysanenko^a, Karolína Fárníková^a, Jozef Lengyel^{*b}, Eva Pluhařová^{*a}, and Michal Fárník^{*a}

^a *J. Heyrovský Institute of Physical Chemistry, v.v.i.,*

The Czech Academy of Sciences; Dolejškova 2155/3, 182 23 Prague 8,

Czech Republic. Fax: +420 2 8658 2307; Tel: +420 2 6605 3206;

E-mail: michal.farnik@jh-inst.cas.cz, eva.pluharova@jh-inst.cas.cz

^b *Chair of Physical Chemistry, Department of Chemistry and Catalysis Research Center,*

Technical University of Munich, 85748 Garching,

Germany. E-mail: jozef.lengyel@tum.de

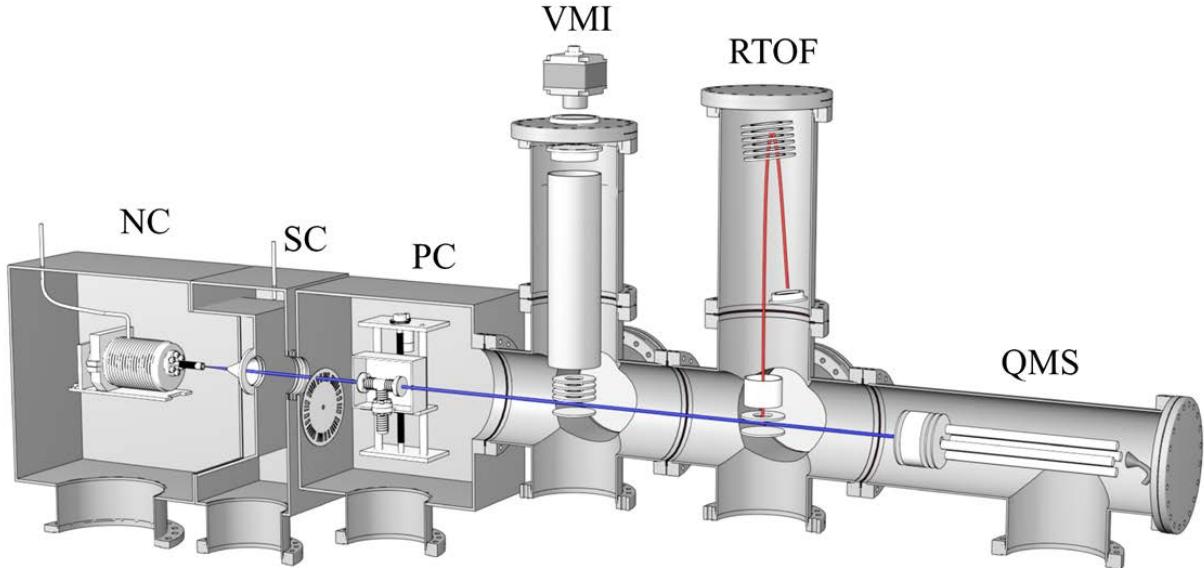


FIG. S1. Schematic drawing of the experimental apparatus CLUB. NC-nozzle chamber, where the mixed nitric acid-water clusters are produced by supersonic expansion; SC-scattering chamber used as a pickup chamber to dope the clusters with dimethylamine molecules; PC chamber with a chopper and another pickup oven, which were not implemented in the present experiments; VMI-velocity map imaging experiment, which was not implemented in the present experiments; RTOF-reflectron time-of-flight mass spectrometer, which was exploited in the present experiments; QMS-quadrupol mass spectrometer.

I. EXPERIMENTAL RESULTS

A. Positive ion mass spectra pickup pressure dependence

Figure S2 shows the positive ion mass spectra of the $(\text{HNO}_3)_M(\text{H}_2\text{O})_N$ clusters after the pickup of DMA molecules and the evolution of the spectra with increasing p_c pressure of DMA in the pickup chamber. It extends Fig. 1 in the main article by showing some intermediate p_c pressures not shown in the main article.

B. Negative ion mass spectra

The negative ion mass spectrum presented in the main article in Fig. 2a) differs slightly from our previously published mass spectra of negatively charged $\text{HNO}_3\text{-H}_2\text{O}$ clusters [1,

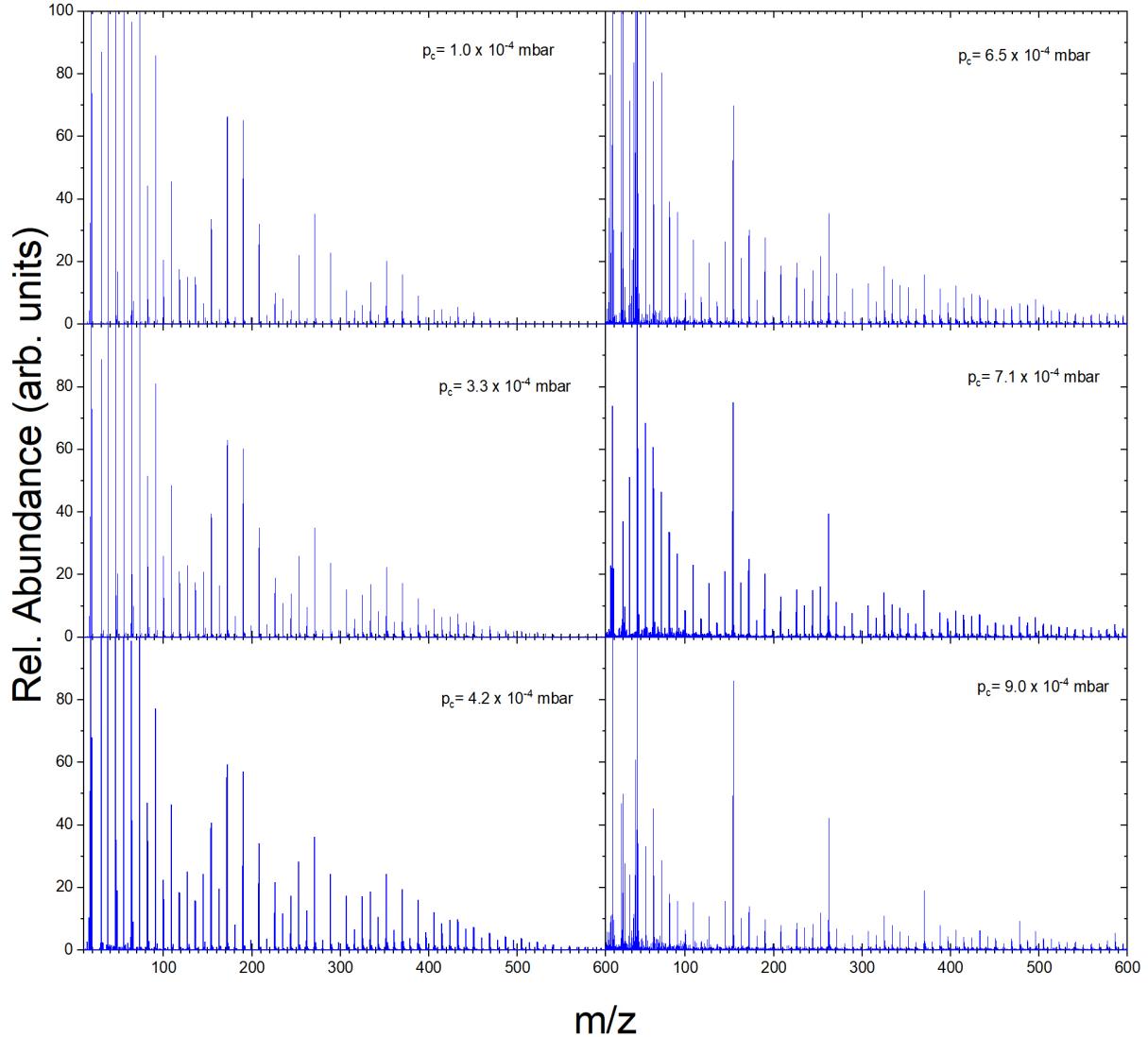


FIG. S2. Mass spectra of $(\text{HNO}_3)_M(\text{H}_2\text{O})_N$ clusters after the pickup of DMA molecules. The panels show the spectra evolution with increasing pressure p_c of DMA in the pickup chamber.

2]. The present spectrum exhibits qualitatively the same mass peaks but with somewhat different intensities: the ratio of integrated intensities of the ion series containing NO_2^- and NO_3^- is 1.0 ± 0.1 (we do not discuss the other minor series, since they are not of concern here). The difference from our previous experiments is due to the different expansion conditions outlined in the Experiment section of the main article. In the present experiments, somewhat higher buffer gas pressure of 3 bar has been used compared to 1 bar and 2 bar used previously. Thus, more diluted $\text{HNO}_3/\text{H}_2\text{O}$ vapor leads to the generation of slightly smaller (and less hydrated) clusters, which in turn can lead to the situation closer to the isolated HNO_3 , which

is dominated by the generation NO_2^- ion. However, our focus here is on the qualitative change of the spectra, when the DMA molecules are added, which is discussed in the main article.

C. Hydrated clusters in the negative ion spectrum

Figure S3 shows a detail section of Fig. 2 in the main article. In the lower panel of Fig. S3b), there is a series of 3 peaks (light green open triangles down) following the $\text{DMA}\cdot\text{HNO}_3\cdot\text{NO}_3^-$ that are displaced by 18 u and thus could correspond to the series $\text{DMA}\cdot\text{HNO}_3\cdot(\text{H}_2\text{O})_n\text{NO}_3^-$. However, these peaks also coincide with the original series $(\text{HNO}_3)_2(\text{H}_2\text{O})_n\text{NO}_3^-$ in the top panel Fig. S3a). We can compare the intensities of $\text{HNO}_3\cdot(\text{H}_2\text{O})_n\text{NO}_3^-$ and $\text{HNO}_3\cdot(\text{H}_2\text{O})_n\text{NO}_2^-$ series in panel (a) and (b), and consider the intensity of $(\text{HNO}_3)_2(\text{H}_2\text{O})_n\text{NO}_2^-$ series in panel (b) (first member labeled by the purple opened circle). This comparison can give us an estimate of the contribution of the original $(\text{HNO}_3)_2(\text{H}_2\text{O})_n\text{NO}_3^-$ series in the coinciding mass peaks. Based on this comparison, we can assume that more than half of intensity in the coinciding series is due to the original $(\text{HNO}_3)_2(\text{H}_2\text{O})_n\text{NO}_3^-$ ions and not due to the hydrated $\text{DMA}\cdot\text{HNO}_3\cdot(\text{H}_2\text{O})_n\text{NO}_3^-$ series. Analogical arguments can be put forward for the series of 3 peaks following the $\text{DMA}\cdot(\text{HNO}_3)_2\text{NO}_3^-$ peak (light green closed triangles down) and spaced by 18 u, and for other small peaks which could be considered due to the hydrated clusters with DMA. In summary, the hydrated cluster ions $(\text{DMA})_k(\text{HNO}_3)_m(\text{H}_2\text{O})_n\text{NO}_3^-$ might be present in the negative ion spectrum of the DMA doped clusters, but their abundance is significantly lower than the population of the non-hydrated ions.

D. Negative cluster ion energy dependence

First, due to the mass coincidence, we have to exclude any significant contribution from the pure clusters to the DMA-doped ones: e.g., $(\text{HNO}_3)_1(\text{H}_2\text{O})_6\text{NO}_3^-$ could contribute to $(\text{DMA})_1(\text{HNO}_3)_2\text{NO}_3^-$ at $m/z = 233$. However, this contribution could be estimated from the neighbouring $(\text{HNO}_3)_1(\text{H}_2\text{O})_n\text{NO}_3^-$ peaks and the character of the pure spectrum without pickup to be below 1% for all the peaks, where the masses coincide. Thus the spectra in Fig. 3 in the main article are clearly due to the electron attachment to the DMA-containing clusters.

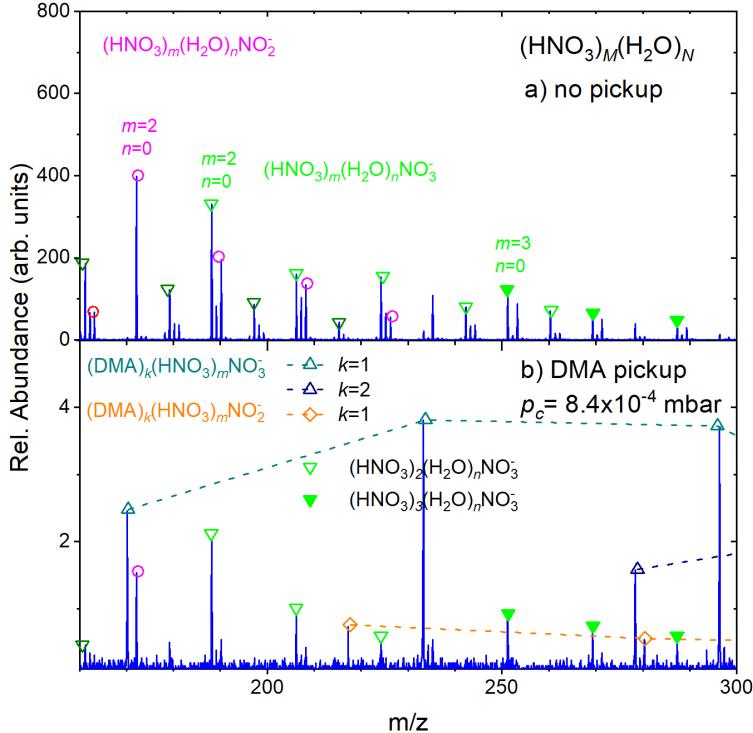


FIG. S3. Detail of the mass spectra of Fig. 2 in the main article. Light green triangles down in panel (b) indicate the series that could be assigned to hydrated clusters $\text{DMA}\cdot\text{HNO}_3\cdot(\text{H}_2\text{O})_n\text{NO}_3^-$ (open) and $\text{DMA}\cdot(\text{HNO}_3)_2(\text{H}_2\text{O})_n\text{NO}_3^-$ (closed). However, they coincide with the $(\text{HNO}_3)_2(\text{H}_2\text{O})_n\text{NO}_3^-$ and $(\text{HNO}_3)_3(\text{H}_2\text{O})_n\text{NO}_3^-$ series, respectively, in the spectrum without pickup (a) labeled by the same symbols.

In our previous works,[1, 2] we have discussed that the low energy resonance below 3.5 eV in the NO_3^- containing ions can be due to two different mechanisms: either (1) the HNO_3 acidic dissociation in water yields $\text{NO}_3^- \cdots \text{H}_3\text{O}^+$ ion pair within the cluster, and the attached electron reacts with the H_3O^+ ; or (2) the dissociative electron attachment (DEA) to HNO_3 yields NO_2^- or OH^- as in the gas phase and subsequent ion-molecule reactions within the cluster convert them to NO_3^- . Based on the dominance of NO_2^- ions over NO_3^- at the energies below 3.5 eV [2], we have put forward the latter mechanism as the more probable one. In the present study, the cluster ions with NO_2^- exhibit abundances too low to evaluate any E_e -dependence. Nevertheless, the cluster ions with NO_3^- dominate even at low energies, which could be consistent with the former ion-pair mechanism: $\text{DMA}\cdot\text{H}^+ \cdots \text{NO}_3^-$ in the present case. On the other hand, the similarity of the low energy resonance below 3.5 eV in pure and DMA-doped clusters suggests similar mechanism in these species. Thus we cannot

make any unambiguous conclusion about the exact mechanism of the electron attachment to the doped $(DMA)_K(HNO_3)_M(H_2O)_N$ clusters at the low energies below 3.5 eV.

Two less pronounced features were observed in the energy spectra of the electron attachment to the pure $(HNO_3)_M(H_2O)_N$ clusters [2]: the NO_3^- containing clusters exhibited broad bands around 6 eV and 11 eV. Two processes have been considered to contribute here: either (1) the reactions initiated by DEA to water, or (2) a selfscavenging mechanism, where the electrons undergo an inelastic collision with a cluster constituent and the slow electrons react further [3]. Unfortunately, the signals of the clusters after the pickup are orders of magnitude lower than the pure $(HNO_3)_M(H_2O)_N$ cluster signals, and consequently the present energy spectra with DMA have a much worse signal-to-noise ratio. Therefore, it is difficult to claim the presence of the higher energy bands unambiguously, nevertheless, they seem to be present in the $DMA \cdot (HNO_3)_m NO_3^-$ spectra and diminish in the spectra with more DMA. If these higher energy bands were due to the DEA to water, the spectra in Fig. 3 in the main text might indicate that there is still some water left in the clusters with DMA at the moment of the electron attachment, and that there is less water in the clusters with more DMA molecules. Although this is a very tentative observation, it seems to be consistent with the mass spectra above, which suggest also some small contribution of hydrated $(DMA)_k(HNO_3)_m(H_2O)_n NO_3^-$ mass peaks.

II. COMPUTATIONAL RESULTS

A. Positively charged clusters

Figure S4 shows optimized structures of the $DMA_2(HNO_3)_2(H_2O)_n H^+$, $n = 0 - 3$ clusters. The DMA moieties are always present in the protonated form. The $n = 0 - 2$ structures contain one HNO_3 and one NO_3^- moiety. The third water molecule (Fig. S4 bottom right) promotes acidic dissociation of the HNO_3 , so the cluster consists of two $DMA \cdot H^+$, two NO_3^- , two H_2O and one H_3O^+ .

B. Negatively charged clusters

Figure S5 shows that the cost of evaporation of a water molecule from the negatively charged $DMA_k(HNO_3)_m(H_2O)_n NO_3^-$ or $DMA_k(HNO_3)_m(H_2O)_n NO_2^-$ clusters is usually be-

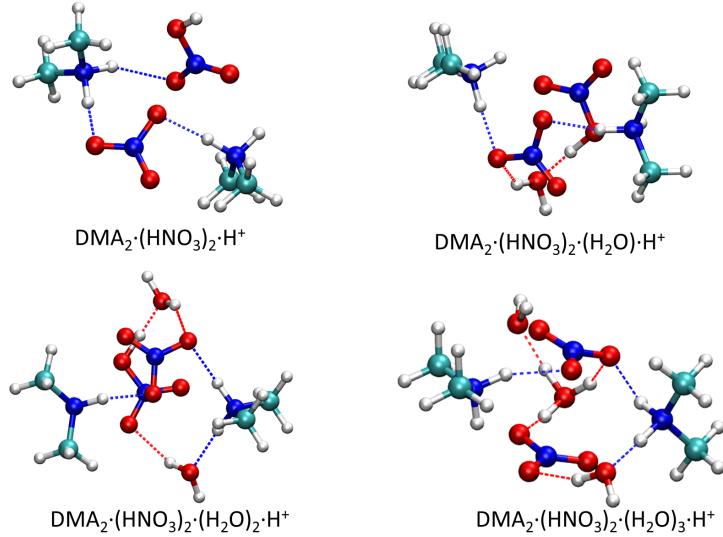


FIG. S4. Structures of $\text{DMA}_2(\text{HNO}_3)_2(\text{H}_2\text{O})_n\text{H}^+$, $n = 0 - 3$ clusters.

tween 40 - 60 kJ/mol.

Figure S6 indicates that the dehydrated negatively charged clusters adopt planar arrangement (the beginning of each row). Increasing hydration leads to the 3D structures. The $\text{DMA}_2(\text{HNO}_3)_2(\text{H}_2\text{O})_{0-4}\text{NO}_3^-$ structures contain only $\text{DMA}\cdot\text{H}^+$ and NO_3^- moieties. The next row with $\text{DMA}_2(\text{HNO}_3)_2(\text{H}_2\text{O})_{0-2}\text{NO}_2^-$ illustrates the fact that HONO is a weaker acid than HNO_3 . If water is absent, the cluster has two NO_3^- surrounding $\text{DMA}\cdot\text{H}^+$ and one neutral DMA hydrogen-bonded to HONO. Addition of water molecules stabilize the $\text{DMA}\cdot\text{H}^+ \cdots \text{NO}_2^-$ ion pair. The last two rows illustrate that $\text{DMA}_k(\text{HNO}_3)_m(\text{H}_2\text{O})_n\text{NO}_3^-$ or $\text{DMA}_k(\text{HNO}_3)_m(\text{H}_2\text{O})_n\text{NO}_2^-$ with $k < m$ possess a neutral molecule of nitric or nitrous acid, resp. in addition to the $\text{DMA}\cdot\text{H}^+$ and NO_3^- moieties.

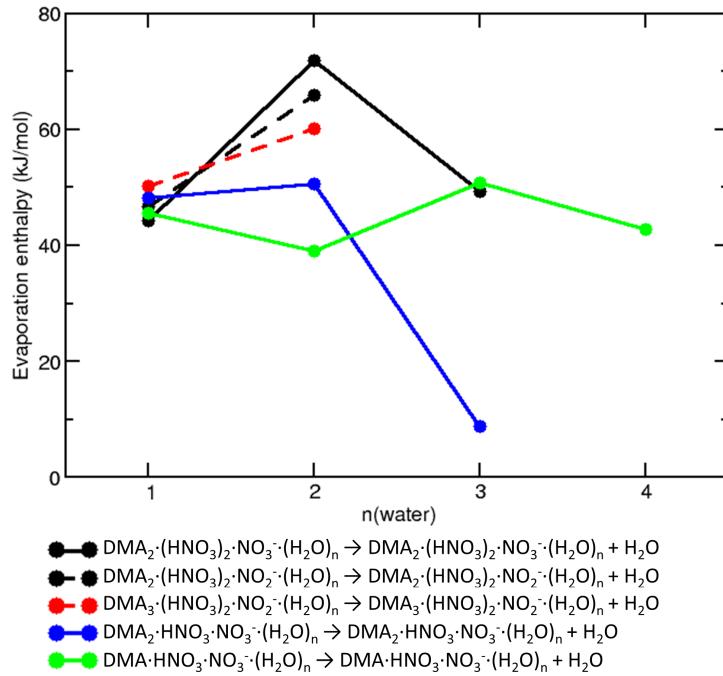


FIG. S5. Binding enthalpies of H₂O in the DMA_k(HNO₃)_m(H₂O)_nNO₃⁻ (solid lines) or DMA_k(HNO₃)_m(H₂O)_nNO₂⁻ (dashed lines) structures as a function of number of water molecules. Different colours correspond to different cluster composition.

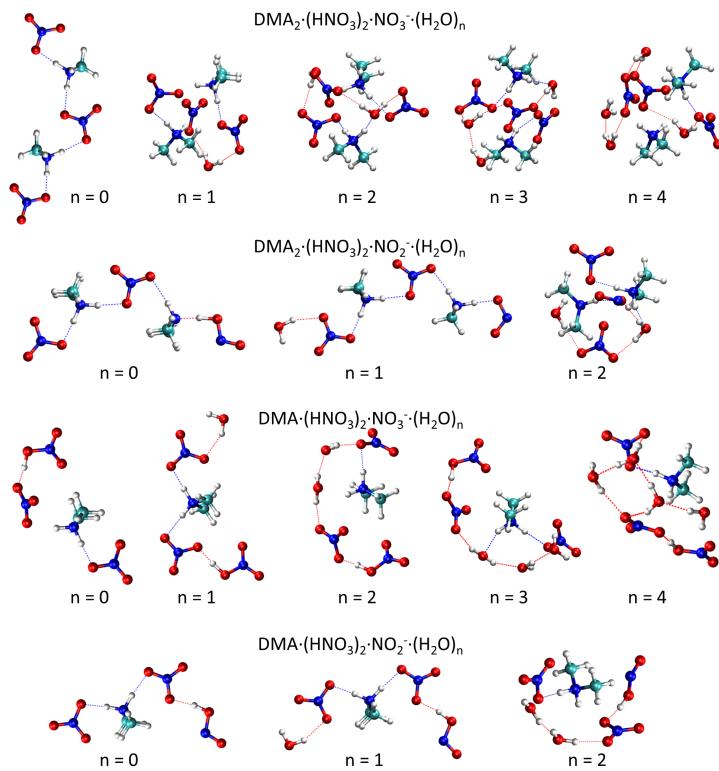
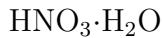
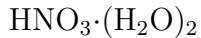


FIG. S6. Optimized structures of $\text{DMA}_2(\text{HNO}_3)_2(\text{H}_2\text{O})_{0-4}\text{NO}_3^-$ (1st row), $\text{DMA}_2(\text{HNO}_3)_2(\text{H}_2\text{O})_{0-2}\text{NO}_2^-$ (2nd row), $\text{DMA}(\text{HNO}_3)_2(\text{H}_2\text{O})_{0-4}\text{NO}_3^-$ (3rd row) and $\text{DMA}(\text{HNO}_3)_2(\text{H}_2\text{O})_{0-2}\text{NO}_2^-$ (4th row).

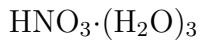
C. XYZ coordinates of structures used for calculations



N 0.835277 0.070487 -0.001887
O 0.225075 1.123350 0.004765
O 2.019067 -0.086919 -0.019634
O 0.102086 -1.066177 0.012091
H -0.850359 -0.767592 0.019377
O -2.341577 -0.029414 0.077772
H -2.005705 0.874281 0.001312
H -3.016893 -0.129065 -0.601085



N -1.319673 -0.194439 -0.001705
O -2.483714 -0.466830 0.022337
O -0.386412 -0.981527 -0.002883
O -1.025155 1.110328 -0.032370
H -0.008785 1.193500 -0.039357
O 1.515931 1.457885 -0.072619
H 2.009158 0.608877 -0.043647
H 1.880322 2.010285 0.625719
H 2.954558 -1.532971 -0.606393
O 2.480365 -1.060308 0.084589
H 1.575406 -1.402967 0.067933



O 0.252564 2.221588 0.000581
O -1.878462 0.872331 0.092949
N -1.524315 -0.402744 -0.048978
O -2.398038 -1.216386 0.044349
O -0.339786 -0.623658 -0.262685
O 2.496821 0.776141 0.000824
H -1.002559 1.422599 0.048516
H 0.405738 2.872483 0.692083

H 1.061001 1.648647 -0.026288
H 2.378754 -0.191911 0.086275
H 3.069317 0.893035 -0.763134
H 1.089249 -1.937560 -0.033579
O 2.052952 -1.950939 0.063916
H 2.237115 -2.545569 0.796705

HNO₃·(H₂O)₄

O -0.780741 -0.777275 -1.425262
O 1.541830 -1.081612 -0.649950
N 1.913129 -0.155092 0.211696
O 1.115686 0.757192 0.453227
O 2.999723 -0.267248 0.697506
O -2.643299 -1.495935 0.369458
O -1.673640 0.779572 1.521123
H 0.532446 -0.898070 -0.947370
H -1.457538 -1.180744 -0.832530
H -1.029577 0.158203 -1.508345
H -2.409365 -0.767607 0.981044
H -2.755542 -2.288915 0.899992
H -0.717715 0.672793 1.615229
H -1.750725 1.382886 0.767368
O -0.916897 1.997453 -1.003962
H -0.015091 1.882349 -0.664993
H -0.930095 2.827574 -1.489383

HNO₃·(H₂O)₅

O 1.309802 -1.912702 0.092838
O -1.073091 -1.884817 -0.406382
N -1.580388 -0.770420 0.050849
O -2.636536 -0.403214 -0.406553
O -0.951099 -0.160160 0.915418
O 2.090573 -0.125038 -1.786667
O 1.790838 0.059657 1.911523

O 1.213784 1.966612 -0.150592
 H -0.006456 -1.913262 -0.114668
 H 1.710131 -1.445275 -0.671807
 H 1.516285 -1.316719 0.851220
 H 1.861808 0.703920 -1.327406
 H 2.923824 0.031108 -2.238854
 H 1.639126 2.824945 -0.060447
 H 0.250352 2.157898 -0.234352
 H 1.557187 0.767180 1.283562
 H 1.029877 0.014273 2.501377
 O -1.458038 2.411264 -0.150734
 H -1.683856 1.663083 0.424628
 H -2.025432 2.292970 -0.920013
 HNO₃·(H₂O)₃·H⁺
 O -0.915683 -1.099864 -0.120757
 O -3.140358 -1.454073 0.961938
 N -3.501943 -2.690404 0.786509
 O -4.569596 -3.002040 1.324220
 O -2.817664 -3.443965 0.139470
 O -6.299422 -6.840863 2.299193
 O -5.066317 -5.370520 0.731877
 H -2.223793 -1.321100 0.479637
 H -0.550434 -0.217727 -0.259810
 H -0.609007 -1.661325 -0.842572
 H -5.569272 -5.964286 1.426947
 H -6.206958 -6.862968 3.259403
 H -4.866025 -4.377360 1.008387
 H -4.265383 -5.792961 0.388146
 H -7.191067 -7.141015 2.082942
 HNO₃·(H₂O)₄·H⁺
 O -15.177510 1.352890 -11.180235
 O -11.572988 -0.857338 -11.917225

N -10.682433 -0.806094 -11.072644
O -9.508846 -0.803025 -11.295406
O -11.111327 -0.749099 -9.816827
O -14.042772 -0.919054 -11.205270
O -8.994735 -0.566149 -8.442048
O -15.324802 -2.613068 -12.592968
H -15.184922 2.025709 -11.869983
H -15.560816 1.746358 -10.388358
H -14.479165 -0.003581 -11.220416
H -13.054241 -0.881338 -11.416704
H -14.533488 -1.597667 -11.781662
H -10.267921 -0.704110 -9.227036
H -8.185051 -0.695115 -8.951189
H -15.758859 -3.376822 -12.195506
H -15.168124 -2.826174 -13.520063
H -8.835073 -0.902050 -7.552774

HNO₃·(H₂O)₅·H⁺
O -4.469658 -0.298963 3.361522
O -6.457389 -1.725497 2.770372
O -7.194240 -1.542148 0.313746
O -6.145256 0.707932 5.368457
N -6.077964 1.665434 6.127310
O -4.910032 2.290330 6.125241
O -6.956222 2.060390 6.844063
O -5.205531 4.242739 7.713898
H -3.562519 -0.613927 3.440458
H -4.673542 0.225586 4.152778
H -5.607549 -1.183971 2.973254
H -6.760699 -1.617467 1.818398
H -7.193656 -1.485128 3.445484
H -4.997951 3.072022 6.786837
H -6.003064 4.221224 8.256083

H -7.561851 -0.786277 -0.156552

H -7.253091 -2.301079 -0.276851

H -4.521547 4.696047 8.219494

H -7.784637 -0.356350 5.072804

O -8.176001 -1.000915 4.461527

H -8.739441 -1.590379 4.974835

DMA·HNO₃·H₂O

C 5.105253 6.524426 7.205947

N 5.881380 7.707860 7.626761

C 5.107235 8.960254 7.637245

O 7.859363 7.965622 5.988592

N 8.598241 6.931242 6.115973

O 8.235637 6.050931 6.938915

O 9.602368 6.815863 5.452508

O 7.518198 6.524558 9.517679

H 6.737151 7.810967 6.942029

H 6.303142 7.516814 8.546715

H 4.257726 6.374754 7.882598

H 4.745767 6.689678 6.185490

H 5.773927 5.660995 7.225452

H 5.759371 9.779070 7.952761

H 4.744723 9.156525 6.623545

H 4.257913 8.872640 8.322652

H 8.006843 6.287559 8.704087

H 8.144678 6.475386 10.243660

DMA·HNO₃·(H₂O)₂

C 5.091425 5.545219 6.709306

N 5.995813 6.593481 7.215812

C 5.327515 7.807345 7.726833

O 8.315068 7.296716 6.038528

N 8.853962 6.209156 6.446775

O 9.945011 6.252888 7.006629

O 8.219702 5.153120 6.310977
H 6.697848 6.863468 6.487709
H 6.616113 6.220150 7.973926
H 4.440690 5.208456 7.521968
H 4.486349 5.956689 5.895829
H 5.708182 4.722302 6.341406
H 6.101344 8.499884 8.072056
H 4.741997 8.262520 6.922613
H 4.670947 7.532011 8.557554
O 7.852778 6.140697 9.187420
H 8.544780 5.549292 8.859616
H 8.240498 7.034679 9.097995
O 8.543156 8.711188 8.360331
H 9.377261 9.106771 8.630630
H 8.694316 8.383994 7.448597

DMA·HNO₃·(H₂O)₃

N -4.724581 10.453238 8.509178
C -4.862106 9.113115 7.913132
C -3.435373 11.124554 8.251536
O -6.432077 12.356321 7.771577
O -5.103820 13.683864 9.855824
H -3.466030 12.108891 8.728683
H -3.305695 11.239813 7.171309
H -2.619440 10.524523 8.665582
H -4.791746 9.197856 6.824554
H -4.064224 8.464262 8.287342
H -5.836992 8.714806 8.203341
H -5.493910 11.101941 8.161814
H -4.900465 10.423234 9.531898
H -5.380240 14.507881 10.267356
H -5.286997 12.987291 10.516849
H -7.384248 12.172979 7.924628

H -6.162991 13.021770 8.431290
O -8.981247 11.517652 8.420080
H -9.350877 12.137646 9.059015
H -8.573554 10.845120 8.996069
N -6.796083 11.110580 10.665322
O -7.131697 10.106280 9.999530
O -7.604236 11.978593 10.973179
O -5.575594 11.233271 10.990188

DMA·HNO₃·(H₂O)₄

C 7.573675 -1.410010 -16.041536
N 6.957919 -0.114813 -15.698127
C 6.856298 0.144863 -14.248891
O 8.954067 1.664218 -16.380499
O 9.553006 -0.226299 -18.364527
O 7.021426 0.697990 -18.651762
O 7.225053 3.380185 -17.814900
O 4.438808 2.081227 -18.168976
N 4.772724 1.548023 -17.115435
O 4.537159 0.333535 -16.902105
O 5.411430 2.197586 -16.242962
H 6.976117 4.130182 -18.362161
H 6.454330 3.202312 -17.227646
H 10.144346 -0.237972 -19.122067
H 9.413674 1.153396 -17.069774
H 6.120720 0.517133 -18.949313
H 8.665266 -0.012420 -18.711515
H 7.061012 1.668296 -18.548424
H 8.615907 2.455441 -16.829234
H 7.544273 0.642120 -16.110704
H 6.007185 -0.033428 -16.127293
H 6.998170 -2.216691 -15.577926
H 7.571376 -1.515601 -17.128174

H 8.605508 -1.421513 -15.678006
H 6.359093 1.108642 -14.119562
H 6.267778 -0.650189 -13.781525
H 7.864005 0.171904 -13.823932

DMA·HNO₃·(H₂O)₅

O 10.448131 1.913828 -10.306105
O 7.766451 2.465087 -9.522652
O 7.688339 1.465374 -7.025258
O 6.053395 3.547382 -11.407115
O 8.878675 3.938772 -12.163439
N 9.020651 4.622878 -11.156375
O 10.077863 4.573351 -10.483365
O 8.087849 5.371850 -10.749668
O 10.173138 2.604884 -7.567603
H 10.803279 1.389440 -11.028810
H 10.518623 2.852265 -10.584876
H 6.305943 3.215711 -12.275958
H 6.583799 4.361599 -11.326871
H 7.356997 0.573959 -6.888214
H 9.483234 2.004820 -7.232684
H 7.116472 2.704095 -10.215392
H 7.532585 1.678538 -7.970083
H 8.561078 2.138244 -9.977439
H 10.489300 2.194183 -8.388342
H 9.154974 3.937837 -8.088908
N 8.648806 4.849798 -8.046296
C 7.470755 4.693320 -7.171667
C 9.614973 5.867013 -7.587436
H 8.356042 5.073795 -9.016879
H 6.970994 5.660780 -7.065996
H 6.799468 3.962466 -7.626087
H 7.800924 4.325868 -6.195763

H 10.424629 5.909282 -8.319070

H 9.113009 6.836625 -7.519734

H 9.999789 5.567709 -6.608285

DMA·HNO₃·(H₂O)₃·H⁺

C 14.336431 -0.405686 -3.640240

N 15.102141 -0.092437 -2.408983

C 14.269699 0.412521 -1.290060

O 18.741976 1.917548 -3.872035

N 17.775611 1.854674 -4.611920

O 17.899886 2.314359 -5.841158

O 16.691811 1.403053 -4.324357

O 17.644267 0.870152 -1.397423

O 16.917752 -1.815562 -1.313209

O 20.319234 3.052395 -6.127589

H 15.835167 0.596878 -2.617737

H 15.631543 -0.921976 -2.078635

H 13.588420 -1.166589 -3.403278

H 13.849295 0.506682 -3.993870

H 15.028088 -0.774766 -4.400181

H 14.922263 0.606398 -0.436118

H 13.769613 1.331904 -1.605738

H 13.528743 -0.348412 -1.032138

H 17.898645 1.404665 -0.637100

H 18.168045 1.217806 -2.137768

H 20.863870 3.183365 -5.343296

H 18.864943 2.638792 -5.943206

H 17.270801 -2.661958 -1.024190

H 17.583142 -1.132059 -1.144337

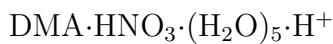
H 20.642023 3.653893 -6.808052

DMA·HNO₃·(H₂O)₄·H⁺

C -6.785595 3.871818 -13.022944

N -7.397410 2.612617 -13.504615

C -8.608544 2.196324 -12.757739
O -8.110697 1.316994 -15.905216
O -5.780256 -0.269550 -16.192589
O -6.000032 0.249362 -13.439691
N -6.061672 3.103990 -16.483015
O -6.806311 4.027385 -16.234716
O -5.445221 2.447955 -15.673861
O -5.896424 2.746426 -17.750816
O -7.392134 4.321673 -19.101177
H -7.219881 4.607882 -20.005661
H -7.663058 5.103031 -18.604534
H -5.210477 0.452019 -16.494642
H -8.884428 1.164452 -16.456234
H -5.384855 -0.174261 -12.833509
H -5.533822 -1.050353 -16.700491
H -5.809362 -0.104650 -14.325311
H -7.490056 0.596530 -16.106114
H -7.634417 2.679922 -14.501880
H -6.711846 1.830010 -13.461619
H -7.505848 4.685252 -13.143069
H -6.526010 3.753274 -11.967543
H -5.891955 4.070921 -13.616941
H -8.979814 1.271581 -13.204167
H -8.335770 2.029393 -11.712361
H -9.361403 2.986125 -12.826771
H -6.474612 3.376825 -18.307608



C 5.991425 5.832336 -9.415535
N 5.989855 4.401952 -9.019483
C 5.648162 4.168162 -7.598170
O 8.494091 3.186886 -10.165618
O 6.565189 1.380081 -9.432634

O 5.311570 0.359533 -11.489134
O 6.663466 1.076825 -13.494407
O 2.943315 1.127813 -11.449505
O 4.734827 2.947957 -13.042010
N 5.126519 3.323238 -11.938335
O 6.329269 3.552095 -11.718521
O 4.298430 3.455360 -10.991747
H 3.030033 2.099905 -11.428318
H 2.330025 0.909303 -12.160459
H 6.770354 0.559690 -14.300535
H 6.225326 1.913875 -13.735095
H 6.821666 0.695718 -8.802856
H 7.390720 1.832156 -9.700206
H 5.836383 0.586758 -12.344358
H 5.775510 0.754626 -10.691828
H 4.305475 0.649472 -11.527783
H 9.457126 3.196774 -10.137896
H 8.234671 3.346470 -11.085425
H 6.905798 3.996008 -9.246116
H 6.728225 6.371387 -8.814078
H 6.243923 5.888211 -10.476950
H 4.992369 6.241214 -9.243824
H 5.658020 3.092337 -7.411703
H 6.380791 4.674004 -6.963515
H 4.650582 4.572883 -7.408041
H 5.318827 3.908472 -9.649933

DMA₂·HNO₃·H₂O

C 4.705249 7.425715 6.974128
N 5.356011 6.181790 7.390060
C 5.349166 5.989259 8.838516
N 7.927361 5.906840 6.574530
C 8.575191 5.029097 7.565912

C 8.580800 7.210252 6.377912
O 6.291630 6.438579 4.330604
N 5.822984 5.310921 4.554434
O 6.634988 4.345005 4.734265
O 4.612393 5.115095 4.652622
H 4.886184 5.389545 6.951581
H 3.679437 7.503000 7.367548
H 5.283756 8.278901 7.354119
H 4.682390 7.463178 5.880955
H 5.758939 4.999722 9.066629
H 5.972332 6.761367 9.311536
H 4.336265 6.064181 9.265163
H 7.823292 5.403745 5.675365
H 8.023689 7.752045 5.609683
H 8.565069 7.761690 7.324368
H 9.618080 7.064650 6.057831
H 8.611508 5.548406 8.529495
H 7.974669 4.118112 7.655063
H 9.592775 4.787372 7.241860
H 6.877471 6.060945 6.878972
O 5.837863 3.256694 7.099775
H 5.242506 2.502335 7.100164
H 5.999944 3.455545 6.153381

DMA₂·HNO₃·(H₂O)₂

C 10.156532 15.454865 0.401031
N 9.800164 16.063344 1.677540
C 8.609506 16.897942 1.588296
O 12.075212 17.175749 2.628135
N 11.906049 17.375746 5.253055
C 10.573140 17.998082 5.383359
C 12.979025 18.132575 5.930704
O 12.215351 14.556090 4.999699

N 11.254482 14.522878 4.195599
O 10.186196 15.075479 4.497160
O 11.379368 13.952546 3.094090
O 13.676424 14.876336 1.895228
H 11.005337 14.780790 0.555481
H 9.324812 14.883629 -0.043885
H 10.453274 16.240752 -0.305903
H 9.667694 15.333643 2.375853
H 8.340119 17.260111 2.586623
H 7.744184 16.360416 1.165162
H 8.819120 17.765871 0.949732
H 12.764177 16.579426 2.294344
H 11.210126 16.801274 2.268776
H 12.965504 14.365726 2.336515
H 13.888739 14.396901 1.090081
H 12.108904 17.277149 4.203559
H 11.879070 16.398731 5.582748
H 13.020008 19.134958 5.493770
H 12.749934 18.204436 6.998599
H 13.923711 17.613014 5.760505
H 10.615641 18.997183 4.939421
H 10.303739 18.070045 6.441403
H 9.852280 17.371075 4.856274

DMA₂·HNO₃·(H₂O)₃

C 10.498425 14.532826 0.422732
N 10.605962 15.582354 1.450374
C 10.066159 16.890624 1.045505
H 9.020020 16.782890 0.741502
H 10.139971 17.561200 1.904672
H 10.656972 17.270860 0.205104
H 9.443902 14.327610 0.216583
H 11.001972 14.874616 -0.487769

H 10.982893 13.632144 0.807993
H 11.656467 15.714739 1.707054
H 10.130771 15.267872 2.304332
N 13.269142 15.963539 1.873535
C 13.572587 17.251940 2.495005
C 13.990436 15.757124 0.622242
H 15.080020 15.874293 0.738657
H 13.786387 14.749282 0.243265
H 13.650688 16.489320 -0.123668
H 13.206209 18.064232 1.852811
H 13.072271 17.313923 3.466127
H 14.654378 17.394992 2.646819
H 13.500533 15.222791 2.538040
O 13.291892 14.447667 4.389292
N 12.165535 13.927499 4.227268
O 11.360721 13.862606 5.164160
O 11.852564 13.490215 3.094648
O 10.474829 16.448519 4.120185
H 11.192452 16.708558 4.727509
H 10.189559 15.600026 4.486024
O 12.698216 16.725390 5.829115
H 12.457036 16.580150 6.748829
H 13.012363 15.854525 5.512458
O 9.116640 13.791607 3.105530
H 9.992912 13.400957 3.292514
H 8.593008 13.619407 3.893060

DMA₂·HNO₃·(H₂O)₄

C 10.142406 9.723663 0.596371
N 10.869791 8.772281 1.433242
C 12.163753 8.417933 0.858457
O 12.525734 7.827546 4.200044
O 8.255943 8.109633 2.605106

N 8.763075 7.809161 3.684407
O 9.762949 7.072081 3.753311
O 8.274295 8.277067 4.758672
O 13.083646 10.541589 4.522582
O 10.559018 10.165299 3.819263
O 7.852188 10.868404 3.818067
N 10.654650 8.381852 6.157021
C 10.613627 7.107611 6.899732
C 10.949631 9.567512 6.981348
H 12.152055 10.675031 4.239472
H 11.368500 8.284139 5.400531
H 7.734803 9.966649 4.173849
H 7.430935 10.824385 2.953822
H 13.595563 11.257415 4.137739
H 9.676899 10.577796 3.750750
H 10.688572 9.645955 2.982046
H 11.813975 7.743596 3.547614
H 12.926335 8.703569 4.057828
H 10.291256 7.943195 1.559327
H 10.025911 9.371928 -0.442001
H 9.149792 9.888264 1.027587
H 10.685993 10.677441 0.578795
H 12.642754 7.636504 1.458274
H 12.080305 8.061771 -0.182059
H 12.815448 9.301583 0.864995
H 9.745828 8.490209 5.657098
H 10.370898 6.318448 6.184194
H 11.592528 6.925715 7.352933
H 9.843012 7.166778 7.674009
H 11.946342 9.459790 7.419016
H 10.924536 10.446575 6.334713
H 10.197637 9.651715 7.771690

DMA₂·HNO₃·(H₂O)₅

C 0.591082 5.004132 21.088247
N 0.869215 3.588129 21.322473
C 1.450224 2.943130 20.146230
O 3.050723 3.176959 23.001724
O 6.011426 4.672764 20.329735
N 5.067752 4.878319 21.132600
O 3.925324 5.069534 20.723376
O 5.311716 4.853793 22.365897
O 7.230205 1.501034 19.674690
O 5.967047 -0.442293 21.231471
O 4.627033 1.872640 21.293094
O 4.947384 2.881208 18.640198
H 4.406832 3.135079 17.887642
H 5.258803 3.716394 19.054438
H 6.549391 1.854247 19.079840
H 6.979752 2.411266 21.190747
H 4.441973 2.196300 20.397709
H 3.976450 2.301247 21.907157
H 6.880805 0.644554 19.977925
H 5.304720 0.279591 21.317012
H 5.472836 -1.246822 21.054568
H 3.572207 3.994322 22.980787
H 2.215148 3.386960 22.516558
H 0.011057 3.110739 21.581676
H -0.065714 5.169975 20.217134
H 0.118282 5.436927 21.976476
H 1.542408 5.519498 20.914100
H 1.641846 1.885548 20.361691
H 0.802714 3.016916 19.255695
H 2.405651 3.433869 19.923167
N 7.247535 2.843237 22.100319

C 8.552078 3.503800 21.902096

C 7.246645 1.799939 23.143824

H 6.528962 3.565289 22.303787

H 7.598121 2.234369 24.084396

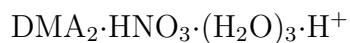
H 6.227960 1.423639 23.253546

H 7.903894 0.984188 22.829442

H 8.867049 3.969327 22.840606

H 9.280370 2.751986 21.585003

H 8.424890 4.261157 21.125624



N -6.299734 5.787703 -1.208460

H -7.140943 5.328511 -0.799381

H -6.669869 6.436278 -1.926232

C -5.506304 4.748396 -1.908224

C -5.543325 6.524628 -0.172072

H -4.661528 5.226007 -2.411790

H -5.146263 4.023794 -1.172748

H -6.159017 4.262384 -2.636591

H -6.200036 7.266220 0.289121

H -5.192628 5.815335 0.582556

H -4.688588 7.021394 -0.639191

O -8.681980 4.763667 -2.499462

N -9.232980 4.369732 -1.465782

O -8.613422 4.446984 -0.365452

O -10.374585 3.896738 -1.480812

N -12.543866 2.500701 -0.279401

H -12.357063 2.348271 -1.285601

C -13.291151 1.356530 0.287662

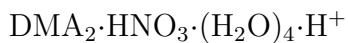
C -13.254673 3.795774 -0.147661

H -11.631378 2.596638 0.208297

H -13.456736 1.538619 1.353164

H -14.250837 1.265116 -0.228290

H -12.705165 0.444240 0.151911
H -12.623749 4.571743 -0.585466
H -14.206482 3.732596 -0.681498
H -13.420834 3.995817 0.914136
O -7.410243 7.070013 -3.402988
H -8.189466 6.511544 -3.526962
H -7.505610 7.828244 -3.986741
O -10.394938 3.072161 1.340227
H -9.714371 3.566351 0.845497
H -9.977056 2.740404 2.139520
O -12.239181 2.698019 -3.034506
H -12.326610 2.305982 -3.907862
H -11.418813 3.215029 -3.027860



C 5.075183 9.506350 4.544787
N 5.220347 10.751795 5.330212
C 4.047747 11.070192 6.175847
O 6.194216 12.690689 3.602898
O 8.776992 13.003223 4.479981
O 10.826277 14.452809 5.773147
N 8.146834 15.169843 6.517710
C 7.722653 16.095137 5.445526
C 8.192566 15.782429 7.865633
O 8.629982 12.606402 7.596048
N 7.648888 12.103508 7.027827
O 7.659761 10.905322 6.692383
O 6.648057 12.813891 6.765405
O 10.691862 11.710022 6.107268
H 11.030362 13.519844 5.976995
H 9.083082 14.792365 6.293430
H 11.245337 10.923027 6.107221
H 10.100344 11.650663 6.879748

H 11.642939 14.944539 5.904871
H 9.457519 13.622173 4.186091
H 9.293502 12.284210 4.884988
H 6.155523 12.709312 2.641834
H 7.137387 12.795352 3.840989
H 5.430728 11.540926 4.685313
H 4.207642 9.597656 3.885250
H 5.981321 9.356601 3.952748
H 4.933523 8.665952 5.229716
H 4.263610 11.989522 6.723148
H 3.171177 11.199278 5.535115
H 3.879929 10.245008 6.873486
H 7.514538 14.345380 6.549980
H 7.196013 16.153207 8.119842
H 8.502093 15.011247 8.574061
H 8.908079 16.609293 7.856585
H 8.446914 16.910798 5.368556
H 7.673542 15.539657 4.506080
H 6.735514 16.495720 5.690936
H 6.075123 10.700863 5.922079

DMA₂·HNO₃·(H₂O)₅·H⁺
C 4.133517 3.445423 8.316151
N 4.803857 4.522044 9.079206
C 4.545042 4.477496 10.534510
O 7.520625 4.854533 8.739113
O 4.454794 7.073775 7.966057
N 4.999941 6.885241 6.849116
O 5.132778 7.819091 6.060573
O 5.429466 5.741834 6.564869
O 7.371969 9.708012 5.751708
O 9.765310 8.657990 6.460934
O 5.899464 9.541103 8.164063

O 7.728457 7.413179 7.843012
N 7.533827 6.806176 4.994846
C 8.810439 6.061062 5.062245
C 7.031636 7.026628 3.619682
H 5.716352 10.212167 8.829135
H 5.091971 9.006245 8.071384
H 7.027296 10.329071 5.102215
H 6.734153 9.721330 6.491539
H 7.163262 8.122899 8.192597
H 7.632373 5.788370 8.456533
H 9.171633 9.378711 6.188754
H 8.571447 7.840161 7.604791
H 10.618954 9.054131 6.661523
H 8.231920 4.673303 9.360647
H 5.832738 4.500588 8.912228
H 4.526427 5.448402 8.695403
H 3.053581 3.519676 8.471458
H 4.373976 3.578566 7.259925
H 4.494895 2.477639 8.674595
H 5.084103 5.298849 11.012972
H 3.471080 4.581821 10.711651
H 4.894542 3.520271 10.931493
H 7.617496 7.722967 5.457451
H 9.072056 5.917452 6.112074
H 8.673351 5.094367 4.570424
H 9.589096 6.640907 4.562130
H 7.769704 7.611326 3.063760
H 6.883670 6.056872 3.137106
H 6.083408 7.563214 3.691745
H 6.806233 6.308314 5.543087

DMA₂·(HNO₃)₂·H⁺

N 0.245921 -4.186629 1.101059

C 0.743158 -4.582051 2.444287
C 0.136857 -5.325799 0.150736
H -0.255432 -4.946985 -0.796467
H -0.550754 -6.053192 0.588384
H 1.126551 -5.767351 0.007924
H 0.044233 -5.313942 2.853434
H 1.742776 -5.011904 2.337964
H 0.774903 -3.697359 3.084570
H -0.705982 -3.761414 1.174879
H 0.849720 -3.470160 0.694600
C -6.057354 -3.295813 -1.508933
N -4.914481 -2.816622 -0.695730
C -5.187814 -1.566084 0.051997
H -5.764114 -4.211082 -2.028466
H -6.894588 -3.503215 -0.837342
H -6.338574 -2.524083 -2.230862
H -5.370736 -0.750314 -0.652717
H -6.069223 -1.727837 0.678186
H -4.320057 -1.353660 0.680374
H -4.632452 -3.547388 0.021733
H -4.088750 -2.688149 -1.287006
N -2.955313 -4.310470 1.410526
O -4.168709 -4.515191 1.219211
O -2.284437 -5.049731 2.117091
O -2.406000 -3.311355 0.846154
N -1.494257 -2.231532 -1.412168
O -2.061434 -3.089523 -2.019910
O -2.240752 -1.104142 -1.212236
O -0.377489 -2.228327 -0.960165
H -1.662540 -0.506099 -0.705155

DMA₂·(HNO₃)₂·H₂O·H⁺

N 0.086363 -4.150216 0.946678

C 0.555691 -3.008716 1.771314
C 0.653538 -5.462421 1.346676
H 0.264056 -6.226946 0.672897
H 0.335010 -5.676423 2.370011
H 1.743896 -5.406698 1.292199
H 0.264748 -3.191098 2.809075
H 1.643464 -2.935714 1.693495
H 0.085366 -2.097023 1.396551
H -0.953452 -4.186162 0.990096
H 0.290097 -3.960885 -0.039078
C -5.905500 -2.234246 -1.469734
N -5.016610 -2.533773 -0.320927
C -5.614231 -2.251881 1.006488
H -5.369412 -2.468456 -2.392142
H -6.801714 -2.854187 -1.383289
H -6.178857 -1.176052 -1.445902
H -5.858464 -1.188505 1.073948
H -6.521859 -2.852365 1.109353
H -4.887887 -2.533191 1.772257
H -4.724288 -3.539296 -0.344714
H -4.134620 -2.026142 -0.429934
N -3.044297 -5.036996 0.368535
O -4.145621 -5.149872 -0.233362
O -2.273354 -5.982125 0.446756
O -2.739073 -3.915557 0.856138
N -1.682685 -3.075482 -1.609833
O -2.808327 -2.866002 -2.009289
O -0.962345 -2.292532 -1.039702
O -1.172585 -4.293025 -1.788060
O -2.946615 -5.848786 -2.606056
H -1.918783 -4.919192 -2.191052
H -2.674428 -6.732425 -2.879633

H -3.557689 -5.955146 -1.852392

DMA₂·(HNO₃)₂·(H₂O)₂·H⁺

C 0.009273 -4.413038 1.316850

N 0.490584 -3.175723 1.979234

C 1.697387 -3.364656 2.821329

O 0.853441 -0.256855 1.990892

N -0.303764 0.021115 1.725239

O -0.966351 0.880334 2.254626

O -0.852391 -0.719691 0.777698

O -3.268790 -0.218576 0.604051

O -3.245258 -1.035136 3.198847

N -2.361539 -1.903312 2.989032

O -1.278380 -1.822795 3.632619

O -2.524508 -2.783706 2.154627

O 0.902510 0.533093 4.747191

N -1.900366 0.693141 5.000289

C -2.356681 2.100709 4.979672

C -2.189805 -0.021526 6.265185

H -0.272742 -5.129262 2.092734

H 0.813085 -4.820281 0.697790

H -0.865041 -4.163919 0.713545

H -0.264222 -2.775973 2.583152

H 0.673858 -2.447416 1.283130

H 1.467588 -4.108740 3.588327

H 2.523547 -3.711716 2.195464

H 1.944274 -2.407883 3.287343

H -0.879169 0.655894 4.826330

H -2.347018 0.161470 4.231718

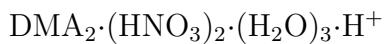
H -2.094397 2.537098 4.013236

H -1.861828 2.647089 5.787272

H -3.440074 2.125233 5.124261

H -3.270315 -0.022363 6.431848

H -1.681965 0.489146 7.087831
 H -1.821168 -1.044789 6.164915
 H -3.637941 -0.525320 1.457276
 H 1.133905 0.467710 3.808417
 H 1.573150 1.092924 5.151414
 H -1.886620 -0.455297 0.678159
 H -3.751193 -0.676059 -0.094914



C 0.065066 -4.040721 0.940445
 N 0.549136 -3.148037 2.020342
 C 1.630739 -3.721948 2.856391
 O -4.018970 -2.852280 0.092008
 O -3.240119 -0.507590 0.653925
 O -0.805929 -0.859908 0.895610
 N -0.323380 -0.090100 1.794390
 O -1.023950 0.781899 2.288305
 O 0.848714 -0.288308 2.142245
 O -3.257840 -1.117002 3.275526
 N -2.356821 -1.987635 3.164231
 O -2.494895 -2.942769 2.389464
 O -1.306336 -1.863583 3.821546
 N -1.877714 0.792571 4.998398
 C -2.221656 0.168246 6.295763
 C -2.346503 2.188349 4.850836
 O 0.881013 0.644490 4.784529
 H -0.357632 -4.939159 1.396772
 H 0.907373 -4.301323 0.294356
 H -0.702589 -3.506790 0.377498
 H -0.241989 -2.885385 2.633846
 H 0.856575 -2.248193 1.627797
 H 1.260809 -4.635623 3.328719
 H 2.490192 -3.948601 2.220276

H 1.904477 -2.987860 3.618083
H -0.844289 0.762899 4.871176
H -2.273300 0.209112 4.246786
H -2.036184 2.553413 3.869250
H -1.897384 2.797557 5.639998
H -3.436016 2.210868 4.940226
H -3.308751 0.166494 6.412786
H -1.757344 0.743725 7.101124
H -1.839232 -0.854839 6.290817
H -3.493739 -0.506979 1.607985
H 1.053228 0.461970 3.843610
H 1.547900 1.278611 5.065366
H -2.175051 -0.589995 0.691098
H -3.851442 -3.232957 0.969675
H -3.615500 -1.386938 0.297115
H -4.885116 -3.149861 -0.206518

DMA₂·(HNO₃)₂·(H₂O)₄·H⁺
C 0.124458 -4.370205 1.228511
N 0.550918 -3.095001 1.847167
C 1.589932 -3.245520 2.893059
O 0.801105 -0.024622 2.078804
N -0.394706 0.096485 1.770946
O -1.150140 0.857745 2.360799
O -0.835073 -0.620916 0.814523
O -3.290817 -0.333963 0.657784
O -4.140422 -2.630083 0.038624
O -3.304898 -1.116294 3.249072
N -2.370486 -1.939024 3.062522
O -1.308851 -1.811895 3.697974
O -2.492226 -2.849415 2.231062
O 0.813537 0.622712 4.800159
N -1.947826 0.695689 5.077163

C -2.433132 2.092659 5.041451
C -2.262331 -0.028002 6.329276
H -0.304604 -5.010857 2.002927
H 0.997286 -4.848911 0.776510
H -0.628634 -4.151872 0.468307
H -0.264699 -2.637521 2.274766
H 0.924708 -2.465806 1.114707
H 1.211387 -3.913520 3.671001
H 2.491666 -3.657963 2.433804
H 1.795345 -2.257273 3.310642
H -0.917364 0.687172 4.930065
H -2.349065 0.163382 4.290710
H -2.145363 2.531856 4.083617
H -1.975156 2.648073 5.864559
H -3.520944 2.096468 5.152001
H -3.347201 -0.052845 6.463158
H -1.791305 0.491139 7.168358
H -1.868029 -1.042754 6.240607
H -3.518344 -0.364596 1.616925
H 0.972449 0.550492 3.841887
H 1.480367 1.225352 5.143272
H -2.226374 -0.405410 0.657207
H -3.904247 -3.049029 0.883425
H -3.686331 -1.200528 0.281566
H -5.042092 -2.885024 -0.184435
H 1.954219 -0.727904 0.495068
O 2.208441 -1.610855 0.191773
H 2.456643 -1.523439 -0.733674

DMA₂·(HNO₃)₂

N 0.353917 -2.315528 0.144872
O -1.052994 -0.249563 -1.037186
N -2.108061 -0.266648 -0.335340

O -2.513591 -1.332912 0.123755
O -2.694105 0.810398 -0.110185
O 2.692709 -0.810873 0.105574
N 2.106843 0.266177 0.331274
O 2.512495 1.332557 -0.127371
O 1.051785 0.248843 1.033145
N -0.355091 2.314969 -0.148791
H 1.327726 -1.946310 0.173197
H -1.329261 1.946786 -0.176808
H -0.207415 -1.515073 -0.227228
C -0.084829 -2.640585 1.518538
C 0.213926 -3.434438 -0.805099
C -0.213474 3.433807 0.801031
C 0.083496 2.639570 -1.522700
H 0.205637 1.514023 0.223055
H -0.795947 4.289670 0.447334
H -0.575995 3.111904 1.780363
H 0.847243 3.693563 0.865521
H -0.534475 3.457517 -1.905930
H 1.137004 2.926428 -1.491839
H -0.050597 1.744428 -2.132902
H 0.534058 -3.457659 1.902176
H 0.047782 -1.745242 2.128775
H -1.137934 -2.928884 1.487336
H 0.797254 -4.289667 -0.451276
H -0.846461 -3.695423 -0.870045
H 0.576465 -3.112001 -1.784249

DMA₂·(HNO₃)₂·H₂O

C 2.031534 -1.241505 1.576351
N 1.856297 -1.533602 0.138010
C 3.103456 -1.929473 -0.540607
O 1.200125 2.776121 -0.139673

N 1.672309 1.664859 -0.373213
O 0.927788 0.792236 -0.953619
O 2.816720 1.340445 -0.061082
N -1.589286 1.535621 -0.182054
C -1.502456 1.788385 1.272897
C -1.928233 2.740709 -0.963494
O -0.355659 -3.184246 0.174892
N -1.252770 -2.318152 0.249240
O -2.443776 -2.640931 0.154054
O -0.937518 -1.117158 0.417270
O -3.724271 -0.237703 -0.164393
H 1.472826 -0.675395 -0.326292
H -2.301819 0.796623 -0.330834
H 1.104505 -2.254452 0.054338
H -0.665303 1.169201 -0.511920
H -2.477574 2.135404 1.627202
H -1.246165 0.844951 1.759535
H -0.731913 2.543900 1.446170
H -2.900006 3.119446 -0.632285
H -1.142882 3.483880 -0.803644
H -1.972954 2.472471 -2.022286
H 2.754449 -0.428859 1.682217
H 1.056999 -0.948592 1.974284
H 2.383973 -2.145438 2.082274
H 2.882101 -2.144646 -1.589099
H 3.806814 -1.094615 -0.474469
H 3.513363 -2.820977 -0.056257
H -3.320522 -1.119452 0.004224
H -4.504595 -0.406702 -0.698616



N -1.520128 -2.051094 -0.251310
O -0.735738 -2.927484 -0.616736

O -2.709695 -2.054949 -0.601532
O -1.100717 -1.111044 0.492100
O -3.997405 0.037003 0.622916
H -3.616589 -0.768145 0.207422
H -4.604492 -0.284325 1.294494
N -1.727509 1.587377 0.282918
H -2.279350 0.844544 0.735149
H -0.715875 1.422105 0.492056
C -1.927942 1.444252 -1.175966
H -1.314004 2.194992 -1.679487
H -1.621568 0.435282 -1.462233
H -2.989910 1.583331 -1.394952
C -2.150598 2.903992 0.796715
H -1.934314 2.951589 1.867262
H -1.585110 3.677092 0.271482
H -3.225546 3.013324 0.626020
N 1.476146 2.153122 -0.023920
O 2.695546 2.165770 -0.248929
O 0.732816 3.042999 -0.439178
O 0.983126 1.189895 0.640478
N 1.633288 -1.500883 0.406885
H 0.605157 -1.340208 0.514464
H 2.133996 -0.774891 0.938988
C 1.985149 -1.309439 -1.017376
H 1.427753 -2.041100 -1.607331
H 1.709815 -0.290531 -1.299972
H 3.064290 -1.444162 -1.128680
C 2.001702 -2.834983 0.917686
H 3.088756 -2.941058 0.857081
H 1.674394 -2.917938 1.957450
H 1.495339 -3.588719 0.310397
O 3.852740 0.032949 1.034089

H 3.515962 0.852287 0.608455

H 4.382752 0.330324 1.778074

DMA₂·(HNO₃)₂·(H₂O)₃

N -0.521540 -2.987250 1.665237

C 0.137086 -2.872989 0.347556

H 0.240178 -3.873164 -0.082740

H 1.111070 -2.397760 0.486286

H -0.496222 -2.258855 -0.298198

H -1.467208 -3.388115 1.510149

H -0.649425 -2.022387 2.030007

C 0.232901 -3.796156 2.645253

H 0.352408 -4.807953 2.246287

H 1.207083 -3.324118 2.795864

H -0.337735 -3.814964 3.576507

N -2.539043 -2.056581 3.952336

O -1.554074 -1.945472 4.706132

O -3.266045 -1.046452 3.740550

O -2.801860 -3.127698 3.402692

N 0.407556 0.089256 2.437229

O 1.270640 -0.805252 2.426946

O 0.681646 1.247913 2.741497

O -0.794861 -0.221723 2.170232

N -1.661309 1.036049 4.645169

H -0.655470 0.797542 4.607974

H -2.156355 0.260223 4.157614

C -1.934290 2.310554 3.951919

H -1.601864 2.206827 2.917968

H -1.375474 3.111495 4.444278

H -3.008430 2.511745 4.004178

C -2.079144 1.002145 6.061619

H -3.154943 1.191616 6.115735

H -1.526821 1.765309 6.617013

H -1.852168 0.007655 6.451826
 O -3.167855 -1.140399 0.895260
 H -3.460095 -1.122344 1.823886
 H 1.451982 -0.284500 4.643565
 O 0.729212 -0.312844 5.285252
 H 0.254481 -1.132389 5.082290
 H -2.383756 -0.575864 0.906362
 O -2.949856 -3.895060 0.608023
 H -3.481834 -4.169138 1.364873
 H -3.161904 -2.944081 0.522815

$\text{DMA}_3 \cdot (\text{HNO}_3)_3$
 N 0.684765 -1.098235 -2.072618
 O 2.234236 -1.229391 0.112377
 N 3.235675 -0.440136 -0.074346
 O 3.686026 -0.321531 -1.209178
 O 3.678719 0.167192 0.899084
 N 0.858292 0.016203 2.139407
 O 0.692843 1.302385 -0.468759
 N -0.523918 1.478575 -0.393570
 O -1.033260 2.215942 0.456666
 O -1.289787 0.864880 -1.210579
 N -3.742598 0.886452 -0.015757
 O -2.717616 -1.697190 -0.054644
 N -1.742320 -1.346789 0.632866
 O -0.608925 -1.791290 0.418377
 O -1.914614 -0.501345 1.554291
 C 0.321456 -2.467978 -2.482505
 H 1.329851 -1.150537 -1.231351
 H -0.143641 -0.586672 -1.733641
 C 1.327634 -0.303144 -3.139466
 H -3.706984 -0.080214 0.343411
 H 1.328105 -0.252215 1.247901

C 1.330732 1.333170 2.615035
 H -0.155254 0.027201 1.933471
 C 1.134542 -1.094518 3.072728
 C -3.983106 1.848433 1.076554
 H -2.770044 1.009559 -0.398304
 C -4.692448 0.971745 -1.139893
 H 0.656222 -0.887371 4.034656
 H 0.733479 -2.008411 2.628760
 H 2.219175 -1.175157 3.186811
 H 0.819055 1.570763 3.553185
 H 2.411149 1.271815 2.763381
 H 1.095316 2.074651 1.849805
 H -0.343723 -2.421466 -3.350578
 H 1.237847 -3.004647 -2.744760
 H -0.181303 -2.951593 -1.642636
 H 0.642082 -0.231005 -3.990030
 H 1.550803 0.685269 -2.734412
 H 2.258509 -0.796101 -3.429304
 H -5.709427 0.801810 -0.774404
 H -4.618348 1.965279 -1.591345
 H -4.423484 0.207094 -1.872999
 H -4.997133 1.706273 1.462713
 H -3.238293 1.660367 1.850995
 H -3.859507 2.861411 0.684679

$\text{DMA}_3\cdot(\text{HNO}_3)_3\cdot\text{H}_2\text{O}$
 C -0.167707 2.342438 2.516865
 N -0.135806 2.140229 1.051516
 C -0.084127 3.406037 0.289103
 O -2.090664 0.839971 -0.695607
 N -1.254946 0.327538 -1.470650
 O -1.525031 -0.749956 -2.045396

O -0.156366 0.874293 -1.649517
N -2.980967 -1.664537 0.132705
C -4.373469 -1.181657 0.092707
C -2.841641 -3.096485 0.457048
O -0.141039 -1.432202 0.525032
N -0.250577 -0.932503 1.664775
O -1.384034 -0.523680 2.043095
O 0.720177 -0.825993 2.413267
N 1.820747 -1.222793 -1.495070
C 2.964809 -0.696245 -2.264719
C 1.198966 -2.418997 -2.090613
O 4.110343 0.799466 0.937640
N 3.025145 1.392479 0.924627
O 2.082304 0.922109 0.208519
O 2.824009 2.417116 1.577133
H -0.945212 1.592586 0.726825
H 0.731352 1.594399 0.767651
H 2.157795 -1.437825 -0.520326
H -2.510597 -1.447065 -0.771887
H -2.424952 -1.112335 0.833506
H 1.114677 -0.477748 -1.396364
H -4.352684 -0.125411 -0.183140
H -4.933726 -1.755950 -0.651355
H -4.825722 -1.313478 1.080285
H -3.282873 -3.283304 1.440637
H -3.356692 -3.693481 -0.301470
H -1.775618 -3.335179 0.476170
H 0.709829 2.932915 2.789758
H -1.089703 2.870226 2.780740
H -0.134307 1.368178 3.008159
H -0.946192 4.024672 0.557320
H 0.850302 3.910568 0.550242

H -0.104052 3.157972 -0.773810
H 2.619064 -0.383766 -3.254562
H 3.376509 0.151830 -1.712899
H 3.715979 -1.486276 -2.358849
H 1.956020 -3.204939 -2.167328
H 0.383556 -2.736795 -1.438763
H 0.804209 -2.165040 -3.078129
O 2.978837 -1.825198 0.897608
H 2.250081 -1.595808 1.501641
H 3.563341 -1.046917 0.951287

DMA₃·(HNO₃)₃·(H₂O)₂
C 3.517552 -2.040178 1.244300
N 2.768778 -1.837813 -0.013034
C 3.586350 -1.999954 -1.230420
O 1.839501 0.813626 0.281542
N 2.919909 1.474037 0.076973
O 2.836955 2.683348 -0.133076
O 3.990205 0.867945 0.081168
N -0.106793 2.608464 -0.524924
C -0.056615 3.926000 0.141896
C 0.237915 2.651271 -1.960912
O -2.617395 1.608462 0.727411
N -1.886933 0.990708 1.559237
O -0.826637 1.489880 1.932453
O -2.251007 -0.129321 1.963876
N -3.661943 -0.734836 -0.382229
C -4.702411 -1.338541 0.470195
C -4.062186 -0.543984 -1.788843
O -1.021064 -0.002992 -1.032158
N -0.579265 -1.156820 -1.195482
O -1.335406 -2.135363 -0.933301
O 0.560371 -1.354284 -1.610829

H 2.358935 -0.883484 -0.004209
H 1.965292 -2.502341 -0.027391
H -3.355285 0.176906 0.022795
H 0.561581 1.950635 -0.064247
H -1.034870 2.190099 -0.375976
H -2.793896 -1.315978 -0.383626
H -0.754797 4.602982 -0.360202
H -0.347299 3.782911 1.183991
H 0.966895 4.300750 0.072970
H -0.501211 3.260156 -2.490769
H 1.233570 3.092862 -2.051825
H 0.236714 1.625186 -2.334634
H 3.911677 -3.060792 1.258112
H 4.324606 -1.305028 1.288935
H 2.823057 -1.895847 2.076051
H 3.985714 -3.018440 -1.254553
H 2.942492 -1.826508 -2.095479
H 4.396655 -1.267185 -1.201949
H -4.308915 -1.402807 1.486216
H -5.592722 -0.702692 0.452051
H -4.948175 -2.332672 0.085110
H -4.924226 0.128406 -1.831560
H -3.211499 -0.111676 -2.320935
H -4.321451 -1.514305 -2.222252
O 0.693007 -3.610258 0.469439
H 0.445658 -2.913584 1.105158
H 0.036326 -3.481368 -0.232694
O 0.416891 -1.185253 1.832920
H -0.478411 -0.939883 2.118741
H 0.800291 -0.336486 1.565525

DMA₃·(HNO₃)₃·(H₂O)₃

N 4.098449 -0.080889 0.362892

H 4.268409 -0.558530 -0.548902
H 3.074679 -0.114177 0.503718
C 4.539115 1.327299 0.294594
H 4.293032 1.812394 1.241757
H 4.004458 1.812786 -0.524005
H 5.618527 1.351152 0.116734
C 4.705880 -0.843047 1.470729
H 4.400388 -0.377152 2.411811
H 5.794757 -0.827729 1.367959
H 4.336788 -1.870168 1.427740
O 4.268938 -1.575238 -1.951275
H 3.294244 -1.513783 -2.085642
H 4.657101 -1.280341 -2.780089
N 1.244154 -0.197461 -1.613003
O 0.066410 0.082548 -1.353566
O 2.138909 0.674682 -1.504191
O 1.556440 -1.348284 -1.973603
N -1.100594 -2.004163 0.426897
H -1.996373 -1.925052 -0.072900
H -0.586630 -1.124992 0.285519
C -1.409030 -2.156764 1.864282
H -0.464473 -2.179425 2.413588
H -1.972437 -3.084759 1.990120
H -2.010102 -1.299753 2.170663
C -0.322379 -3.126580 -0.131354
H -0.920073 -4.035693 -0.025424
H -0.107883 -2.912172 -1.179667
H 0.615329 -3.203639 0.424755
N 1.073153 0.336759 1.566803
O -0.130900 0.596980 1.642873
O 1.939600 1.182159 1.870943
O 1.447449 -0.794187 1.156132

O -3.617823 -3.065890 -0.186534
H -4.207334 -2.283545 -0.125381
H -4.055322 -3.659461 -0.802283
N -4.266452 0.156902 -0.090917
O -4.543922 1.342307 -0.269553
O -5.123460 -0.734267 -0.140213
O -3.060963 -0.169151 0.151564
N -1.654254 2.156265 -0.248802
H -0.633957 2.032429 -0.173812
H -2.120886 1.237031 -0.077746
C -1.959903 2.610005 -1.619145
H -3.038661 2.762458 -1.701589
H -1.628244 1.833095 -2.312313
H -1.411898 3.538107 -1.806535
C -2.074476 3.105488 0.799470
H -3.159578 3.221848 0.744237
H -1.562995 4.057719 0.631304
H -1.780615 2.689057 1.766158
O 1.044341 2.923702 -0.203965
H 1.353578 2.680389 0.682126
H 1.429597 2.228724 -0.769332

DMA₂·HNO₃·NO₃⁻

C 3.121498 6.957417 8.110417
N 2.818004 6.925366 6.689507
C 3.729035 6.040699 5.980809
O 9.437645 7.962603 11.726297
N 8.977323 7.942034 10.589965
O 9.585918 7.394779 9.646323
O 7.855452 8.487119 10.351907
N 7.485206 8.131112 7.696409
C 7.499057 6.682181 7.417385
C 8.598956 8.844810 7.042820

O 6.321647 8.315356 4.940062

N 5.223530 8.715004 5.369880

O 5.108983 8.982893 6.603733

O 4.247620 8.841127 4.629833

H 2.953744 7.861809 6.312307

H 2.913810 5.971232 8.550746

H 4.175989 7.218673 8.319390

H 2.483285 7.694888 8.611045

H 3.561927 6.125242 4.901872

H 4.794584 6.267578 6.181274

H 3.541665 5.000795 6.286384

H 6.578210 8.519136 7.339280

H 8.520193 9.906795 7.293354

H 9.535951 8.441060 7.435419

H 8.506793 8.710819 5.962039

H 8.440756 6.272544 7.791037

H 6.659249 6.221153 7.945600

H 7.384102 6.539856 6.339057

H 7.570939 8.276921 8.742161

DMA₂·HNO₃·NO₃⁻·H₂O

C 1.111127 3.732108 -0.326471

N 0.897942 2.332489 0.001854

C 0.169783 2.164744 1.253639

O 4.346268 -0.839616 0.413419

N 3.148952 -0.944554 0.167285

O 2.335235 -0.068793 0.599354

O 2.695698 -1.894432 -0.499797

N -0.156078 -1.011796 -0.257464

C -0.182869 -2.045908 0.797524

C -0.252743 -1.571599 -1.621923

O -2.411461 0.489043 0.431890

N -3.356224 -0.357295 0.300406

O -3.088191 -1.470182 -0.190161
O -4.490420 -0.062208 0.657579
H 1.779771 1.828251 0.062409
H 0.138306 4.212475 -0.499333
H 1.632250 4.288698 0.474671
H 1.696789 3.811726 -1.249599
H 0.161039 1.106386 1.533871
H 0.620699 2.736621 2.084784
H -0.871189 2.486675 1.122442
H 0.744444 -0.501987 -0.139278
H -0.115055 -1.543240 1.766597
H -1.129312 -2.586321 0.720031
H 0.684037 -2.696358 0.654918
H -1.190725 -2.129488 -1.685278
H -0.271071 -0.733669 -2.322831
H 0.619130 -2.209549 -1.785988
H -0.962921 -0.367563 -0.091694
O -1.047038 1.562428 -1.914067
H -1.767013 1.348248 -1.302930
H -0.304700 1.791225 -1.312655

DMA₂·HNO₃·NO₃⁻·(H₂O)₂
C 3.516433 5.945348 6.398602
N 4.436072 7.070706 6.261494
C 4.041642 8.194005 7.103690
O 6.644667 6.651620 8.056781
O 5.899420 4.054898 6.731829
N 7.081371 3.834293 7.113475
O 7.337417 3.798677 8.321625
O 7.979556 3.690730 6.261142
N 6.403430 5.403146 4.349648
C 7.439508 6.429490 4.597407
C 6.837479 4.369813 3.390000

O 5.793435 6.916387 1.882517

N 4.627555 7.186402 2.226419

O 3.889677 7.878532 1.536811

O 4.202201 6.718843 3.334269

H 4.424602 7.362736 5.285531

H 3.633853 5.498772 7.393981

H 2.463259 6.245407 6.255262

H 3.761807 5.176431 5.659429

H 4.731258 9.031819 6.948796

H 3.010780 8.536123 6.901691

H 4.111039 7.894206 8.157255

H 6.157916 4.934570 5.249089

H 7.706762 3.858522 3.810245

H 6.017870 3.657958 3.255472

H 7.061580 4.861438 2.440227

H 7.635672 6.938867 3.650223

H 7.050788 7.134649 5.336392

H 8.333743 5.947934 5.000159

H 5.549569 5.879645 3.968494

H 6.607123 5.759643 8.432779

H 5.975804 6.648447 7.341011

O 9.410569 6.139769 7.264083

H 8.537708 6.456538 7.551884

H 9.267768 5.188928 7.155946

DMA₂·HNO₃·NO₃⁻·(H₂O)₃

C 10.674379 8.442132 22.284163

N 11.937231 7.738840 22.084063

C 12.002391 7.137900 20.756025

O 6.253992 0.914832 20.296485

N 7.461334 0.811817 20.069690

O 8.198126 0.085185 20.766731

O 7.988308 1.484735 19.137965

N 9.802618 2.460887 21.154227
C 8.613733 2.829230 21.967950
C 10.100234 3.380774 20.027171
O 10.776563 4.932032 22.675781
N 11.886715 4.375138 22.847207
O 12.008147 3.148143 22.586205
O 12.850123 5.016317 23.261857
O 8.321547 6.000222 20.894866
O 13.902303 9.703275 22.118814
H 12.010325 6.983229 22.763380
H 10.626268 9.296416 21.594773
H 9.797731 7.799953 22.098387
H 10.629416 8.829439 23.308537
H 12.860119 6.456807 20.710356
H 11.082388 6.583288 20.504898
H 12.143529 7.927423 20.005303
H 9.634309 1.510995 20.792744
H 7.781312 3.051131 21.297381
H 8.365105 1.972287 22.597866
H 8.875090 3.695946 22.575604
H 9.191603 3.545091 19.448990
H 10.483179 4.314746 20.441949
H 10.859138 2.907269 19.400024
H 10.643272 2.501475 21.779011
H 13.230443 8.972829 22.164698
H 14.718908 9.285837 22.405130
H 8.997208 5.588684 21.447768
H 7.848998 5.278159 20.451222
O 6.705199 3.913628 19.403003
H 5.838512 3.704862 19.766300
H 7.053388 3.032709 19.148162

DMA₂·HNO₃·NO₂⁻

N -1.599786 -1.145323 -1.027889
O -0.780720 -1.902360 -0.443460
O -1.248676 0.018751 -1.322321
O -2.735557 -1.547500 -1.293193
C 0.910314 0.821807 0.868355
N 1.421289 -0.248569 -0.006211
C 1.895522 0.265990 -1.302964
H 2.252114 -0.579104 -1.899582
H 1.060293 0.753808 -1.812436
H 2.723219 0.954101 -1.107624
H 2.264717 -0.707763 0.489400
H 0.651217 -0.933442 -0.171853
H 1.740050 1.499292 1.088999
H 0.546385 0.367341 1.794698
H 0.087706 1.330694 0.357629
H -3.632037 0.430983 -0.707270
N -3.812405 0.996409 0.120988
H -3.426371 2.942466 0.790420
C -3.191930 2.296029 -0.068318
H -3.593025 2.772098 -0.971399
H -2.092250 2.232832 -0.170093
C -3.220612 0.294618 1.250073
H -3.496828 0.803390 2.185380
H -3.600755 -0.731894 1.284534
H -2.115451 0.251600 1.196772
O 3.574251 -1.265449 1.187357
N 4.431865 -0.349985 1.341896
O 4.092678 0.768718 0.938374



C -0.341112 -0.894817 1.734973
N -0.030107 -1.136921 0.314653
C 0.121591 -2.567607 -0.002274

O -1.897748 -0.720773 -1.636767
N -2.863242 -1.455591 -1.318010
O -2.964503 -1.690599 -0.097265
O 2.282485 0.325462 -0.114449
N 3.133715 -0.277573 0.611582
O 4.267754 0.174765 0.726432
O 2.780610 -1.323299 1.192096
N -0.255387 1.886476 -0.452685
C -1.033339 2.466745 -1.539821
C 0.224777 2.882104 0.494208
H -1.313188 -1.344522 1.955153
H 0.462073 -1.330484 2.335811
H -0.400576 0.184218 1.895003
H 0.956365 -2.964773 0.581069
H -0.821931 -3.069393 0.232823
H 0.329142 -2.662499 -1.071722
H 0.857872 -0.630823 0.093255
H -0.798844 -0.765997 -0.303813
H 0.546693 1.385020 -0.823434
H -1.932739 2.936465 -1.119325
H -0.472064 3.233627 -2.105502
H -1.357371 1.667534 -2.214687
H 0.924710 2.406163 1.189587
H 0.743150 3.727392 0.005002
H -0.628956 3.279759 1.061065
O -2.674968 1.069501 0.940805
H -1.851865 1.205718 0.435901
H -2.948216 0.180055 0.665849



C 0.217138 -1.441035 -1.794249
N 0.290727 -0.912110 -0.414962
C -0.290110 -1.841997 0.576477

O 2.914228 -0.593235 0.086371
N 3.483731 -1.725594 -0.020022
O 2.721343 -2.679783 -0.166243
O -1.806948 0.728219 1.784731
N -2.510980 0.208327 0.902568
O -2.245302 0.458135 -0.311648
O -3.439706 -0.554715 1.185224
O -3.285577 -1.897226 -1.445256
C 0.412863 3.625014 -0.086634
N 0.355639 2.214483 0.264411
C 1.224105 1.891381 1.389943
H 0.829817 -2.346800 -1.826090
H -0.828303 -1.666015 -2.027914
H 0.628689 -0.682623 -2.465081
H -0.303589 -1.350237 1.552838
H -1.310393 -2.091714 0.268066
H 0.347155 -2.729877 0.600768
H -0.214419 -0.018636 -0.374284
H 1.325524 -0.753936 -0.176547
H -0.599340 1.950159 0.503975
H 2.273940 1.981870 1.081729
H 1.046102 2.545575 2.262201
H 1.056224 0.854499 1.699666
H -0.296007 3.830754 -0.896759
H 0.180057 4.288250 0.766944
H 1.422385 3.867415 -0.445916
H -3.761005 -2.092621 -0.629458
H -2.990426 -0.987830 -1.253905
O 2.022065 1.312591 -1.883658
H 1.358524 1.576575 -1.213692
H 2.628336 0.746814 -1.381985



O 2.497779 -2.513795 -0.174227
O 2.175760 -3.723230 -1.936462
N 2.244468 -2.619426 -1.418789
O 2.066676 -1.567949 -2.072090
N 2.924431 0.099717 0.238978
H 2.657238 -0.911233 0.051787
H 2.094926 0.722707 0.065529
C 3.342904 0.235107 1.643969
H 4.212912 -0.406731 1.818015
H 3.582992 1.284073 1.837794
H 2.519128 -0.086126 2.287065
C 3.980144 0.480239 -0.718982
H 4.260429 1.520177 -0.530328
H 4.834979 -0.191075 -0.583803
H 3.576585 0.358453 -1.726197
N -0.333359 -0.881178 -0.273738
H 0.539830 -0.699566 -0.765471
H -1.390375 0.447285 -0.465349
C -0.853591 -2.166220 -0.745268
H -0.906183 -2.154582 -1.839100
H -1.859944 -2.307656 -0.332925
H -0.212822 -3.008025 -0.434878
C -0.109326 -0.894336 1.170355
H 0.243263 0.094677 1.489904
H 0.618035 -1.668426 1.468487
H -1.067236 -1.098199 1.664003
N 1.309675 2.945191 0.012208
O 0.839518 1.792509 -0.251901
O 0.593066 3.933078 -0.137510
O 2.479894 3.033063 0.419347
N -4.526769 -0.764420 0.443355
O -3.433021 -0.874301 1.039611

O -4.600666 0.041793 -0.535331
 O -5.511772 -1.409770 0.781383
 N -2.148977 1.202038 -0.534302
 C -1.946025 2.024488 -1.737931
 H -3.063673 0.681991 -0.596758
 C -2.191127 1.997804 0.706719
 H -2.826347 2.659231 -1.887912
 H -1.050899 2.637399 -1.599837
 H -1.823264 1.361079 -2.599205
 H -1.271786 2.584322 0.783598
 H -3.061218 2.662903 0.665644
 H -2.305867 1.304028 1.542874

DMA₃·(HNO₃)₂·NO₃⁻·H₂O
 C 0.250158 0.924873 -1.220900
 N 0.008122 0.865063 0.219595
 C -0.513352 2.136087 0.727814
 N -1.781998 -1.226684 0.432796
 C -1.573584 -2.072756 1.620567
 C -1.818012 -1.997910 -0.825388
 O -4.320855 -0.121935 0.360358
 N -4.206874 0.713073 -0.593784
 O -3.083231 0.882538 -1.098729
 O -5.194818 1.325551 -0.991240
 O 2.828940 2.513357 0.212639
 N 2.550276 2.569304 1.455239
 O 2.458736 3.651540 2.012350
 O 2.370436 1.491692 2.064488
 O -7.197830 -0.021911 0.735889
 N 3.298845 -0.078936 -0.278945
 C 4.348993 -0.478072 0.677765
 C 3.726729 -0.181919 -1.683874
 O 2.853830 -3.006200 -0.524619

N 1.677248 -2.927139 -0.136633
O 0.959441 -3.918022 -0.014846
H -1.026819 -0.459309 0.378788
H -2.691608 -0.721459 0.502666
H -2.447825 -2.718508 1.756578
H -1.454772 -1.426392 2.495105
H -0.673408 -2.673845 1.466925
H -1.924527 -1.288085 -1.649112
H -0.897445 -2.581341 -0.906130
H -2.688166 -2.663325 -0.803205
H 0.876651 0.666827 0.713652
H 0.128441 2.985739 0.443503
H -1.518506 2.291711 0.318056
H -0.567486 2.092669 1.820673
H -0.701053 1.141728 -1.721982
H 0.978257 1.710629 -1.483176
H 0.611439 -0.051989 -1.566275
H 3.023467 0.925441 -0.068497
H 2.469631 -0.706860 -0.126755
H 3.939908 -0.373452 1.684737
H 5.205903 0.193580 0.558587
H 4.628917 -1.514913 0.472392
H 2.905735 0.149716 -2.325378
H 3.972284 -1.225449 -1.899114
H 4.595395 0.466520 -1.838722
H -7.148254 0.652243 0.047789
H -6.254736 -0.233529 0.820041
O 1.199895 -1.779160 0.137835



C 2.682349 1.594887 0.856283
N 1.575819 0.708536 1.273261
C 1.344474 0.703857 2.731652

O 2.261113 -1.877220 0.504768
N 3.294936 -2.126476 1.218270
O 3.720782 -1.226174 1.960555
O 0.613836 1.684376 -2.948730
N 0.486843 2.126307 -1.801387
O -0.115761 1.416742 -0.932079
O 0.928363 3.228505 -1.468392
N -0.791227 -0.917934 -2.207102
C 0.537358 -1.546947 -2.337875
C -1.453470 -0.669565 -3.501428
O -2.556063 -2.277061 -0.547430
N -3.294537 -1.272716 -0.261905
O -3.880557 -1.237997 0.814733
O -3.374864 -0.347601 -1.086628
O -0.410324 -1.365734 0.963706
O 0.137242 3.371773 1.437402
N -1.815441 1.287336 1.517026
C -2.809362 2.101751 0.819042
C -2.318455 0.809886 2.800573
H 1.803499 -0.264754 0.966290
H 0.716769 0.995897 0.783183
H -1.425297 -1.493436 -1.606930
H -1.578063 0.484410 0.938613
H -0.657125 -0.007478 -1.708436
H -3.330396 0.382258 2.718808
H -1.651246 0.032702 3.187853
H -2.338706 1.646172 3.514249
H -2.416712 2.371828 -0.166789
H -3.763095 1.568428 0.688805
H -2.977523 3.023132 1.394103
H 2.455067 2.607895 1.194718
H 3.602444 1.204513 1.298389

H 2.747684 1.575342 -0.234828
H 1.051138 1.712849 3.032006
H 0.545383 -0.011597 2.937072
H 2.271177 0.385258 3.214846
H 1.168344 -0.883091 -2.935883
H 0.974032 -1.682399 -1.345488
H 0.426832 -2.517369 -2.831938
H -2.429195 -0.225662 -3.296429
H -0.826091 0.010707 -4.082903
H -1.578572 -1.625608 -4.020753
H 0.295374 3.458633 0.484812
H -0.525239 2.647456 1.498701
H -1.138471 -1.950445 0.694658
H 0.401764 -1.894799 0.924269
O 3.827381 -3.223625 1.145126

DMA₃·(HNO₃)₂·NO₃⁻·(H₂O)₃
C 3.706871 -1.520761 -0.934853
N 2.972719 -1.262363 0.297444
C 3.632983 -1.800889 1.477826
O 0.677284 -0.582027 2.107212
N -0.087137 -1.490332 1.731134
O -1.316343 -1.372238 1.900152
O 0.376972 -2.512916 1.187281
N -2.426520 0.025396 -0.326943
C -2.965629 -0.015018 -1.699678
C -3.361615 0.588214 0.669866
O 0.350444 -0.342747 -1.241654
N 0.527998 -0.675149 -2.442284
O 1.445112 -0.173659 -3.100085
O -0.231721 -1.522790 -2.960511
O -0.694708 2.059281 0.417642
N -0.836800 2.983921 -0.456070

O -1.854656 2.983230 -1.151820
O 0.047680 3.832155 -0.571289
O -0.952593 1.620895 3.238597
O -1.566616 -2.797004 -0.871856
N 1.987644 1.345458 0.371952
C 2.213746 2.100609 1.614952
C 2.652605 1.919697 -0.813942
H 2.041923 -1.678777 0.242461
H 2.314625 0.337308 0.460331
H -1.572441 0.607425 -0.295379
H 0.969132 1.321446 0.210151
H -2.143088 -0.927753 -0.061664
H 1.843693 3.120025 1.467682
H 1.654843 1.617540 2.420119
H 3.286473 2.108302 1.837642
H 2.324518 2.955568 -0.934704
H 3.736653 1.871333 -0.659590
H 2.361090 1.322733 -1.683711
H 4.676403 -1.003833 -0.895499
H 3.903991 -2.596171 -1.091546
H 3.139598 -1.133368 -1.788487
H 4.585366 -1.275275 1.638059
H 2.983448 -1.643441 2.344735
H 3.849252 -2.879896 1.384537
H -3.573034 1.618974 0.371941
H -4.262211 -0.030248 0.681814
H -2.866228 0.570927 1.644108
H -3.219508 1.005525 -1.995688
H -2.197113 -0.429234 -2.357710
H -3.849247 -0.660578 -1.695589
H -1.099310 -2.397407 -1.632310
H -0.889129 -2.869401 -0.176722

H -0.947984 2.066313 2.379711
 H -0.613411 0.741272 3.010977
 O -3.814581 -2.526241 0.744092
 H -3.230346 -2.827998 0.028179
 H -3.177252 -2.358474 1.452391



C 0.894064 -1.436171 -1.214368
 N 2.234135 -1.514085 -0.602854
 C 2.925319 -0.215009 -0.571862
 O 3.748257 -3.116295 -2.096929
 N 3.894109 -2.597212 -3.242226
 O 3.268191 -1.549238 -3.429746
 N 1.541363 -3.639029 1.253030
 C 1.963221 -4.601858 0.240980
 C 2.070721 -3.963815 2.568925
 O 2.739128 -0.780768 2.448682
 N 1.533548 -0.771769 2.683939
 O 0.710392 -0.591983 1.734626
 O 1.087808 -0.955176 3.833476
 C -1.242581 -3.003580 3.583572
 N -1.521416 -1.829133 2.736402
 C -2.068613 -0.689543 3.490473
 O -1.404330 -3.652509 0.470040
 N -2.641295 -3.588551 0.286508
 O -3.199265 -4.248626 -0.574681
 O -3.317498 -2.808187 1.030328
 H 2.832710 -2.192011 -1.197431
 H 2.132435 -1.910977 0.347261
 H -2.203971 -2.142867 1.984099
 H 0.524684 -3.612051 1.267615
 H -0.644627 -1.491306 2.273768
 H 1.723089 -5.643924 0.519301

H 1.474782 -4.379710 -0.713720
H 3.046262 -4.520211 0.083479
H 1.797976 -4.984415 2.901386
H 3.165768 -3.899121 2.536543
H 1.722408 -3.237958 3.311669
H 0.346159 -0.605355 -0.761730
H 1.029232 -1.287826 -2.289779
H 0.355564 -2.368386 -1.017404
H 2.342833 0.476303 0.042469
H 3.911344 -0.357008 -0.122532
H 3.027844 0.130408 -1.604644
H -3.012625 -0.988877 3.957788
H -1.333014 -0.387767 4.241448
H -2.243669 0.135477 2.794827
H -2.177273 -3.315306 4.061641
H -0.883935 -3.810550 2.939693
H -0.490730 -2.732536 4.328959

DMA₃·(HNO₃)₂·NO₂⁻·H₂O

C -1.857552 1.062302 2.943174
N -1.374881 0.764755 1.584021
C -0.052094 1.346827 1.287172
O -2.987865 1.923503 -0.221685
N -4.202153 1.676016 0.062188
O -4.367894 0.953343 1.045228
N -1.449203 -0.332303 -1.471423
C -2.635747 -1.102945 -1.100064
C -1.152491 -0.452243 -2.897250
O 0.486614 -3.351502 2.148871
N -0.092826 -2.260865 2.147691
O -0.796974 -1.933610 1.144676
O 0.022898 -1.459140 3.087336
N 1.124707 -1.430325 -0.974528

C 0.960434 -2.889687 -1.140109
C 2.124607 -1.080908 0.059735
O 3.487712 1.726861 -2.410216
N 2.513996 0.977818 -2.420386
O 2.574774 -0.155910 -2.960280
O 1.433741 1.319386 -1.869085
H -2.085511 1.152558 0.881327
H -1.297032 -0.265867 1.458438
H 1.459260 -1.005438 -1.863275
H -1.656839 0.647051 -1.276824
H 0.181877 -0.995191 -0.798478
H -2.003521 -0.148358 -3.529959
H -0.278974 0.160957 -3.142433
H -0.923920 -1.501390 -3.135798
H -2.409395 -2.174827 -1.173984
H -2.919684 -0.885400 -0.066572
H -3.499191 -0.868169 -1.745523
H -2.839931 0.600199 3.061090
H -1.143186 0.660654 3.666149
H -1.956193 2.148384 3.043906
H 0.696119 0.904872 1.950675
H 0.194926 1.138880 0.241614
H -0.089589 2.430049 1.432714
H 0.155510 -3.069281 -1.857773
H 1.899345 -3.302730 -1.523419
H 0.701782 -3.327127 -0.171777
H 1.833211 -1.522326 1.015038
H 3.089444 -1.490123 -0.255893
H 2.198773 0.006587 0.138608
O 2.628781 2.460862 0.393563
H 2.079299 2.299230 -0.394254
H 3.499550 2.567273 -0.004221

DMA₃·(HNO₃)₂·NO₂⁻·(H₂O)₂

C 2.952182 -1.363034 -0.018563
N 1.565685 -1.744700 0.317332
C 1.445794 -3.093880 0.892991
O 0.348878 -1.088590 -2.007860
N 1.069499 -1.636427 -2.905995
O 1.702426 -2.619250 -2.532612
N -0.848377 -0.667315 2.309053
C -1.631606 -1.720641 2.947914
C -1.309959 0.659411 2.719545
O 1.033811 0.997669 0.567325
N 2.105761 1.652719 0.410535
O 2.940746 1.671445 1.322023
O 2.296537 2.244250 -0.662972
N -0.479867 1.622351 -1.699780
C -0.744405 2.936124 -1.078953
C 0.003481 1.718894 -3.089379
O -2.637505 -0.042412 -1.361918
N -3.128678 0.310057 -0.251316
O -3.150417 1.509066 0.054556
O -3.563832 -0.562343 0.518780
O 1.941120 -0.589936 3.019143
H 0.985771 -1.649257 -0.560333
H 1.206727 -1.053879 0.986031
H -1.337177 1.017084 -1.648960
H -0.984828 -0.766122 1.303074
H 0.230510 1.147086 -1.117006
H -2.715172 -1.579371 2.799418
H -1.346825 -2.691877 2.529844
H -1.417079 -1.723561 4.025674
H -2.376979 0.815451 2.496740
H -1.145527 0.770297 3.800452

H -0.715160 1.418920 2.201995
H 3.496266 -1.179028 0.911532
H 3.397932 -2.173122 -0.600512
H 2.922382 -0.457649 -0.631614
H 2.033610 -3.127007 1.815242
H 0.388019 -3.282007 1.087822
H 1.818738 -3.808841 0.153779
H -0.738992 2.263924 -3.681568
H 0.955178 2.258551 -3.078532
H 0.144242 0.706578 -3.472930
H -1.009011 2.771904 -0.033756
H 0.164945 3.537839 -1.159072
H -1.586478 3.406584 -1.594394
H 2.237474 0.244517 2.620917
H 0.969084 -0.590137 2.876288
O -1.423642 -2.412616 -0.142883
H -2.299445 -2.004490 -0.039937
H -1.102400 -2.041018 -0.979718

DMA₂·NO₃⁻
C -1.788265 1.851008 -0.356645
N -2.250155 0.483996 -0.237986
C -2.480200 0.098293 1.139393
O -0.649946 -2.198634 -0.189281
N 0.325601 -1.825968 -0.868566
O 0.200986 -0.853276 -1.650802
O 1.428640 -2.395111 -0.759991
N 2.445451 0.405090 0.087608
C 2.146258 1.558626 -0.746155
C 1.413125 0.222107 1.100283
H -2.604589 2.545312 -0.100346
H -0.928922 2.087930 0.303754
H -1.483873 2.045881 -1.392054

H -1.622254 0.321995 1.806199
H -3.358976 0.632297 1.535918
H -2.667470 -0.979391 1.183590
H -1.569707 -0.152354 -0.656701
H 0.394376 0.224519 0.674194
H 1.562725 -0.736623 1.609170
H 1.477631 1.031929 1.843649
H 1.145872 1.496931 -1.210436
H 2.895581 1.644053 -1.543599
H 2.195778 2.473040 -0.134516
H 2.421356 -0.425953 -0.503703

DMA₂·NO₃⁻·H₂O

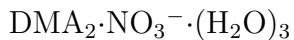
C 2.190245 -1.128286 -0.631989
N 1.132226 -0.557305 -1.456735
C 1.369309 0.855257 -1.709345
O -0.689314 -1.257585 0.949560
N 0.117121 -0.604355 1.636700
O 0.731050 -1.145846 2.573904
O 0.317221 0.606555 1.369388
N -1.867102 1.215576 -0.713489
C -2.183439 0.121849 -1.619756
C -2.804122 1.247885 0.399924
H 1.894911 -2.132490 -0.307014
H 3.113038 -1.211713 -1.225684
H 2.413442 -0.524163 0.266427
H 2.260875 0.965532 -2.344659
H 0.514551 1.291902 -2.241448
H 1.530160 1.433131 -0.780420
H 0.261470 -0.659588 -0.937376
H -2.866200 0.278231 0.927480
H -2.233879 -0.856059 -1.106043
H -3.806576 1.512124 0.029458

H -3.155872 0.315781 -2.097252
 H -1.425039 0.055993 -2.410345
 H -2.488820 2.012414 1.119314
 H -0.950563 1.039730 -0.299273
 O 2.805673 0.826317 2.845574
 H 2.298730 0.012099 3.000082
 H 2.182775 1.267606 2.252444

DMA₂·NO₃⁻·(H₂O)₂

C -1.428106 2.617446 0.734510
 C -1.549363 2.234299 -1.650340
 H -1.158434 2.138714 1.682929
 N -1.344745 1.642555 -0.338005
 H -1.366881 1.471857 -2.413947
 H -2.588230 2.584247 -1.738845
 H -2.459185 2.991057 0.817270
 H -0.877488 3.092141 -1.842037
 H -0.759956 3.486220 0.580673
 H -0.424853 1.198591 -0.317808
 H -3.059724 -1.069945 -0.181760
 O -3.560195 -0.246275 -0.284217
 H -2.839028 0.416939 -0.281704
 N -1.007915 -1.641447 0.342203
 C 0.056494 -2.629608 0.203822
 C -1.039973 -1.086885 1.689299
 H -0.217150 -3.541427 0.754422
 H 1.026226 -2.271486 0.593731
 H 0.180792 -2.884083 -0.854680
 H -0.803023 -0.884241 -0.308369
 H -1.816473 -0.315140 1.747346
 H -0.069566 -0.652412 1.988607
 H -1.297842 -1.885052 2.400392
 O 2.654549 -0.807023 -1.193850

N 1.599915 -0.192601 -0.976211
 O 1.413012 0.373509 0.134728
 O 0.705809 -0.132115 -1.839913
 O 3.443606 -1.064620 1.587924
 H 3.568522 -1.257024 0.647156
 H 2.714641 -0.431548 1.504639



N 1.519336 0.097520 -0.925306
 C 2.787436 -0.400822 -1.438333
 C 1.190088 1.414806 -1.453570
 H 1.605849 0.189951 0.084856
 H 3.023240 -1.356372 -0.954292
 H 3.619214 0.300260 -1.251533
 H 2.701312 -0.571668 -2.520886
 H 2.035994 2.120289 -1.361334
 H 0.922028 1.330312 -2.516524
 H 0.333581 1.822891 -0.906200
 N -3.320646 0.266412 -0.791392
 C -2.197040 0.443461 -1.699802
 C -3.581842 -1.146938 -0.566040
 H -4.340445 -1.262204 0.217876
 H -2.679792 -1.710823 -0.267137
 H -3.974748 -1.597772 -1.489776
 H -2.459559 0.041473 -2.689909
 H -1.976374 1.511631 -1.805690
 H -1.278526 -0.068672 -1.355249
 H -3.035086 0.677735 0.095983
 O 3.416057 1.116313 1.451795
 H 3.205371 0.182821 1.621471
 H 2.562748 1.548531 1.592193
 O 2.002407 -1.368238 1.982795
 H 1.334163 -0.685660 2.177693

H 1.550253 -1.908341 1.311935
 N -0.695189 0.898271 1.432664
 O -1.255489 -0.216658 1.498804
 O -1.298551 1.879925 0.988029
 O 0.494352 1.013462 1.825359
 O 0.143610 -2.229687 -0.041120
 H 0.474155 -1.489908 -0.592806
 H -0.468488 -1.762670 0.551577

DMA₂·NO₃⁻·(H₂O)₄

C 3.207565 -1.742015 -1.164882
 N 2.920107 -0.664837 -0.236047
 C 3.258139 -0.994391 1.136414
 O 0.061605 2.660921 -0.034739
 N 0.141326 1.923301 0.969511
 O 1.214148 1.320418 1.208062
 O -0.840011 1.769760 1.714282
 O 0.410724 -0.025319 -1.871497
 O 2.404438 1.972646 -1.552452
 O -2.053050 0.242541 -0.436036
 N -0.339620 -1.257347 1.138129
 C 0.033211 -2.456854 0.404269
 C -0.719159 -1.512554 2.517396
 H 4.296056 -1.864445 -1.262891
 H 2.784718 -2.714853 -0.846493
 H 2.793810 -1.489368 -2.147186
 H 2.788477 -1.937033 1.482390
 H 4.347476 -1.114859 1.225964
 H 2.937858 -0.178625 1.791700
 H 1.934172 -0.418379 -0.307834
 H -1.638906 -2.113954 2.539103
 H 0.061013 -2.060628 3.078883
 H -0.908468 -0.552245 3.008348

H 0.824732 -3.041237 0.910267
H 0.371596 -2.173387 -0.597691
H -0.849115 -3.100256 0.290246
H 0.415738 -0.571539 1.134767
H 1.748934 2.362180 -0.944618
H 2.849789 1.306237 -1.002048
H -0.378394 0.339987 -1.432834
H 1.024812 0.725813 -1.969852
H -1.537832 -0.313647 0.207520
H -2.074125 1.109398 -0.007640
O -1.830867 -1.729810 -2.550518
H -0.942147 -1.360227 -2.653709
H -2.228333 -1.104033 -1.926976

DMA₃·HNO₃·NO₃⁻

N 0.130664 -0.288450 0.040765
H -0.418039 0.555404 0.345051
H 0.992325 -0.402406 0.634431
C 0.567396 -0.106511 -1.357402
H -0.321495 0.018843 -1.980024
H 1.154914 -0.982567 -1.645901
H 1.188885 0.791975 -1.411176
C -0.731120 -1.473903 0.215408
H -1.616804 -1.348705 -0.413582
H -0.152954 -2.359716 -0.057590
H -1.028608 -1.531668 1.266299
N 2.965455 -1.705093 0.897726
O 2.471591 -0.650289 1.401636
O 2.280959 -2.363452 0.092853
O 4.108267 -2.043089 1.202939
N -2.413182 1.775108 -0.038181
O -1.480694 1.787425 0.812293
O -3.366218 2.545304 0.078489

O -2.354602 0.962752 -0.987300
N 4.897111 0.863212 0.256207
H 4.729691 0.205907 1.016034
C 4.006663 1.998259 0.429302
H 4.222442 2.753018 -0.340931
H 4.173538 2.456487 1.411078
H 2.937754 1.721287 0.357917
C 4.617684 0.164029 -0.987747
H 3.550966 -0.114540 -1.096697
H 5.213929 -0.753009 -1.038557
H 4.887244 0.807409 -1.838126
N -5.234988 0.085768 -0.252517
C -4.940521 -0.979271 -1.194861
H -5.322097 -0.713678 -2.188109
H -3.856687 -1.182955 -1.284675
H -5.442913 -1.903140 -0.872390
C -4.642647 -0.186679 1.047737
H -4.763830 0.686366 1.697596
H -3.562372 -0.424374 0.986771
H -5.152520 -1.043483 1.511951
H -4.814472 0.946964 -0.598068

DMA₃·HNO₃·NO₃⁻·H₂O

C -1.141768 -0.543202 -2.352862
N -0.592624 0.062656 -1.125868
C -0.631041 1.540978 -1.143573
O -2.062600 -0.383676 1.107351
N -3.038207 0.374807 0.826275
O -3.539817 1.070652 1.714898
O -3.450690 0.415540 -0.345555
O 1.866707 -1.312209 -1.266670
N 2.474146 -0.665526 -2.174512
O 3.556701 -1.073716 -2.591392

O 1.948585 0.372523 -2.618750
N 1.422742 0.194508 1.316085
C 1.741919 -0.124877 2.701046
C 2.168277 1.352621 0.835763
N 4.328677 -2.778447 -0.043594
C 3.313536 -3.313433 0.847335
C 4.738599 -1.448343 0.377554
H 0.384752 -0.272030 -1.036138
H -1.133957 -0.264561 -0.285898
H -2.198072 -0.272274 -2.422687
H -1.032500 -1.628580 -2.280074
H -0.563442 -0.171111 -3.203847
H -0.362069 1.908269 -0.149171
H 0.078071 1.890811 -1.898515
H -1.653970 1.848255 -1.377261
H 1.649350 -0.600667 0.723914
H 3.238038 1.317316 1.111657
H 1.730947 2.264019 1.266084
H 2.098460 1.405750 -0.258017
H 2.820801 -0.315713 2.854194
H 1.176252 -1.010348 3.012707
H 1.440474 0.714902 3.340497
H 3.884433 -0.752631 0.475245
H 5.244369 -1.509500 1.352455
H 5.436863 -1.028506 -0.354128
H 3.748169 -3.471866 1.845022
H 2.960313 -4.281170 0.471884
H 2.436631 -2.647321 0.955246
H 3.916805 -2.671943 -0.969520
O -0.704632 1.967853 2.269935
H -1.642674 1.742151 2.356728
H -0.313173 1.151587 1.915333

DMA₃·HNO₃·NO₃⁻·(H₂O)₂

C -0.001987 -1.734421 -0.607494
N 0.518655 -0.432638 -0.136541
C -0.033453 -0.041084 1.177221
O -0.615106 1.098641 -2.325465
N -0.861810 2.188042 -1.759566
O -0.321688 2.429249 -0.652964
O -1.640907 3.000898 -2.270543
O 3.201797 -0.832435 0.042102
N 3.326367 -1.714647 0.937678
O 2.303830 -2.118792 1.532459
O 4.437747 -2.169893 1.204237
O -1.390156 5.072237 -0.201407
C 1.878508 -5.331879 1.294320
N 3.214845 -5.001293 0.831518
C 3.187471 -4.499624 -0.533548
N -3.188503 2.463143 0.426775
C -2.567168 2.687827 1.724982
C -4.607186 2.787744 0.433536
H 0.273514 0.290909 -0.831691
H 1.569463 -0.510310 -0.065521
H -1.093272 -1.678118 -0.634914
H 0.345761 -2.503553 0.087100
H 0.399125 -1.922646 -1.607071
H 0.251553 -0.809641 1.899182
H 0.399363 0.922492 1.454115
H -1.119240 0.044957 1.076318
H 3.583720 -4.254715 1.418187
H 4.180734 -4.130699 -0.810209
H 2.461623 -3.674649 -0.674506
H 2.911409 -5.313975 -1.219172
H 1.912388 -5.627666 2.349799

H 1.489852 -6.181757 0.714263
H 1.170424 -4.487539 1.195064
H -2.971832 1.970005 2.452118
H -1.488305 2.528497 1.633486
H -2.738989 3.710325 2.102664
H -5.133737 2.101684 1.110986
H -5.017635 2.653629 -0.573566
H -4.805949 3.822295 0.766688
H -2.717745 3.057965 -0.252943
H -1.679554 4.996198 -1.118908
H -0.843678 4.272112 -0.131422
O -2.823314 -0.086406 -0.755354
H -2.967130 0.784763 -0.316140
H -2.339253 0.142403 -1.560592

DMA₃·HNO₃·NO₃⁻·(H₂O)₃
C 0.625645 1.028088 1.766773
N 0.232708 0.339790 0.520467
C -0.018314 1.257962 -0.609920
O -3.528193 -2.162911 -0.199722
N -2.432131 -1.640004 -0.000098
O -1.533835 -1.648542 -0.857729
O -2.208091 -1.060050 1.109075
O -2.562846 1.751206 1.670614
N 1.836679 -1.827597 -0.025992
C 1.188454 -2.713825 0.934282
C 1.723503 -2.298164 -1.404272
N 3.643665 0.440368 -0.886392
O 3.175074 1.114952 0.075520
O 3.308418 0.720310 -2.047053
O 4.417012 -0.498403 -0.650785
O 3.514606 -0.581361 2.281685
C -6.114580 0.651060 -0.302412

N -4.697102 0.709073 0.019879
C -3.877947 0.776482 -1.187740
H -0.625269 -0.214628 0.694314
H 0.972696 -0.387806 0.245931
H 1.485896 1.665745 1.553544
H 0.909519 0.274073 2.506691
H -0.221637 1.624063 2.118307
H -0.360798 0.656165 -1.455839
H -0.793155 1.969779 -0.307424
H 0.912360 1.773968 -0.859429
H 2.814871 -1.703489 0.221110
H 1.401607 -2.353255 1.946765
H 1.538768 -3.757195 0.847654
H 0.104336 -2.698899 0.760149
H 2.280674 -1.621254 -2.060771
H 0.664678 -2.297863 -1.690164
H 2.118802 -3.321909 -1.526217
H -4.094171 1.714047 -1.717532
H -2.818455 0.780743 -0.908933
H -4.053063 -0.070981 -1.871779
H -6.416463 1.591486 -0.783925
H -6.700696 0.535322 0.616801
H -6.364101 -0.180317 -0.987284
H -4.444134 -0.151107 0.507049
H 3.422318 0.073207 1.560750
H 4.352616 -0.999726 2.060280
H -3.427594 1.803326 1.228006
H -2.436159 0.790687 1.693753
O 2.683285 3.497458 -1.581134
H 2.835576 2.658772 -2.045399
H 2.853960 3.217340 -0.673620

DMA·HNO₃·NO₃⁻

C 2.150683 -2.231967 4.179317
N 1.581801 -3.587704 4.060193
C 0.784646 -3.972085 5.240307
O -0.133838 -3.536092 1.945176
N -0.997788 -2.663405 2.262788
O -1.921702 -2.409458 1.495824
O -0.881665 -2.080073 3.361488
O 3.687395 -5.311643 3.943591
N 4.303810 -5.129290 5.037042
O 3.855230 -4.285508 5.841837
O 5.317511 -5.775882 5.283397
H 2.725216 -2.020003 3.272625
H 1.324561 -1.521497 4.268567
H 2.812533 -2.214423 5.049288
H -0.046627 -3.268354 5.335043
H 1.441590 -3.962631 6.114117
H 0.397662 -4.982631 5.078635
H 2.377450 -4.273972 3.958994
H 0.952635 -3.610686 3.212970

DMA·HNO₃·NO₃⁻·H₂O

C 1.781256 8.481996 5.102198
N 2.695024 8.573476 6.257489
C 2.032881 9.108394 7.463139
O 1.318538 6.053325 7.072619
N 2.385627 5.396584 7.134455
O 2.382764 4.205845 7.451137
O 3.467713 5.976340 6.865807
O 4.638747 10.318597 5.587262
N 4.024429 11.407968 5.363454
O 4.653059 12.405774 5.029765
O 2.782309 11.427693 5.492506
H 1.428845 9.489928 4.868688

H 2.340293 8.079045 4.252635
H 0.962883 7.805528 5.362273
H 1.216376 8.434688 7.735990
H 1.680381 10.117797 7.236204
H 2.768947 9.146284 8.271488
H 3.495198 9.221730 6.000375
H 3.052313 7.615008 6.473974
O -0.501440 3.907322 7.837183
H 0.391818 3.536377 7.840932
H -0.282382 4.812389 7.572942

DMA·HNO₃·NO₃⁻·(H₂O)₂
C 0.372237 4.662353 8.028610
N 1.837145 4.726928 7.855695
C 2.231354 5.305486 6.555745
O 2.806575 6.405932 9.804436
N 2.238668 7.504342 9.570734
O 2.463101 8.482871 10.278612
O 1.442117 7.572761 8.601467
O 0.675727 10.358539 8.830230
O 1.396044 2.281387 6.232345
N 2.184619 1.591532 6.925797
O 2.766302 2.140206 7.897527
O 2.388313 0.407993 6.667468
H -0.037122 4.024681 7.241127
H 0.160062 4.225105 9.008447
H -0.022534 5.680389 7.983028
H 1.843502 6.325897 6.504049
H 1.829410 4.669919 5.762756
H 3.323697 5.320109 6.502380
H 2.223538 3.752548 7.917886
H 2.237498 5.323826 8.621201
H 0.764746 9.434081 8.547996

H 1.276645 10.352864 9.584609
 O 0.587202 0.266385 4.312496
 H 1.181082 -0.301727 4.817258
 H 0.692149 1.091691 4.812546

$\text{DMA}\cdot\text{HNO}_3\cdot\text{NO}_3^- \cdot (\text{H}_2\text{O})_3$
 C -0.097544 -1.164948 -0.360679
 N -0.246818 -0.822910 1.070918
 C -0.059546 -1.983605 1.957241
 O -3.001679 -1.831312 0.772155
 N -3.458175 -0.696214 0.530885
 O -2.719803 0.310252 0.785541
 O -4.578243 -0.531502 0.066380
 O 3.027855 1.134461 -0.092237
 N 2.880008 -0.107386 -0.275947
 O 2.847690 -0.555887 -1.432273
 O 2.745085 -0.854605 0.705750
 O -0.772722 2.254099 -0.046522
 O 1.087606 1.463020 1.912791
 H 0.959689 -2.355537 1.816965
 H -0.807168 -2.737220 1.695904
 H -0.203389 -1.660398 2.991956
 H -0.094360 -0.234253 -0.934633
 H 0.848158 -1.690516 -0.509942
 H -0.955555 -1.782335 -0.641262
 H 0.413948 -0.062690 1.347608
 H -1.212315 -0.428159 1.173253
 H 0.488652 1.957155 1.321859
 H 1.931810 1.422948 1.427164
 H -0.316043 2.049611 -0.880766
 H -1.579655 1.717427 -0.017188
 O 1.152654 1.739263 -2.077012
 H 1.871980 1.823814 -1.422127

H 1.382003 0.885362 -2.465303
DMA·HNO₃·NO₃⁻·(H₂O)₄
C 0.187952 -0.912866 1.240275
N -0.179720 -1.098467 -0.182340
C -0.076251 -2.500563 -0.624997
O 1.452739 0.592748 -1.741915
N 2.574348 0.208068 -1.307230
O 3.516132 1.001279 -1.237713
O 2.696046 -0.975649 -0.936224
O -2.831778 -0.426016 -0.693410
N -3.357599 -0.787085 0.414352
O -4.311655 -0.151155 0.860590
O -2.873786 -1.761070 1.004456
O -3.138062 2.295599 -0.511648
O -0.384697 1.948670 -0.053201
H -0.794544 -3.089352 -0.047764
H 0.951110 -2.837035 -0.465534
H -0.322173 -2.549059 -1.689386
H -0.467420 -1.548623 1.841043
H 1.241469 -1.175998 1.372319
H 0.031888 0.138258 1.488430
H -1.158004 -0.780702 -0.344639
H 0.431633 -0.504899 -0.776718
H -1.311646 2.207625 -0.214558
H 0.036810 1.812613 -0.912260
H -3.681870 2.298198 0.283951
H -3.159836 1.346874 -0.755849
O 2.200853 2.060160 1.143098
H 1.272651 2.144352 0.870415
H 2.698804 2.064522 0.311979
O 3.481608 -0.450077 1.865074
H 3.041904 0.414045 1.799020

H 3.579816 -0.708756 0.937355

DMA·HNO₃·NO₂⁻

C -0.514235 1.043039 -1.171402

N -0.487943 0.125419 -0.018848

C -0.575588 0.839256 1.267142

O -2.714142 -1.357913 -0.198982

N -3.719230 -0.594536 -0.160807

O -3.467105 0.612329 -0.052848

O 2.359031 0.995325 0.125171

N 2.794514 -0.172767 0.038462

O 4.000754 -0.408412 0.048711

O 1.965137 -1.124650 -0.061556

H 0.412666 -0.413530 -0.041240

H -1.344637 -0.519188 -0.094274

H -0.428571 0.448916 -2.086411

H -1.472994 1.569982 -1.161417

H 0.337125 1.724672 -1.092114

H -1.533728 1.366610 1.295796

H -0.535933 0.101043 2.074009

H 0.277232 1.519157 1.345699

DMA·HNO₃·NO₂⁻·H₂O

C -0.936929 0.566123 1.322569

N -1.010494 -0.027490 -0.024379

C -0.961550 0.989817 -1.089662

O 1.285123 -1.616855 -0.326176

N 2.226682 -0.798441 -0.191949

O 3.396946 -1.175324 -0.269326

O 1.951091 0.409071 0.022226

O -3.392680 -1.187156 -0.204707

N -4.292228 -0.313328 -0.042258

O -3.884476 0.836570 0.156634

O 4.629674 1.472781 0.179863

H -0.023571 1.544986 -1.002695
 H -1.836985 1.635843 -0.976263
 H -1.002205 0.479317 -2.056584
 H 0.001000 1.121089 1.411362
 H -1.812283 1.208933 1.453516
 H -0.960022 -0.243428 2.058303
 H -0.207521 -0.678700 -0.146931
 H -1.958814 -0.545358 -0.105783
 H 3.663149 1.375975 0.173136
 H 4.875919 0.554138 0.017276

DMA·HNO₃·NO₂⁻·(H₂O)₂
 C -0.858313 -1.817097 -0.629589
 N -0.881019 -0.523005 0.067954
 C -0.808685 -0.654958 1.534281
 O 2.056569 -0.651280 0.054401
 N 2.234577 0.468323 -0.483830
 O 1.222482 1.123303 -0.850333
 O 3.363755 0.919079 -0.658565
 O -3.808834 -0.980827 0.384675
 N -4.098633 0.161756 0.026201
 O -3.128965 0.840204 -0.435291
 O -0.986781 2.498733 0.699071
 H 0.122580 -1.167033 1.793837
 H -1.686369 -1.218391 1.865333
 H -0.821694 0.352938 1.957696
 H 0.067041 -2.340394 -0.371676
 H -1.745386 -2.380824 -0.325991
 H -0.889620 -1.633143 -1.707569
 H -0.085140 0.057451 -0.258897
 H -1.791540 -0.011353 -0.173788
 H -0.254525 2.314543 0.095168
 H -1.788077 2.195982 0.245411

O 4.820832 -1.462189 0.345300

H 3.850793 -1.430872 0.367958

H 4.997520 -0.591038 -0.029379

DMA·NO₃⁻

C -4.922236 -0.200974 -0.470634

N -4.241591 0.840124 0.281068

C -4.366836 0.600402 1.710780

O -2.089441 -1.385380 0.391549

N -1.173913 -0.673750 0.861050

O -1.248654 0.573665 0.753822

O -0.200219 -1.194335 1.429341

H -3.241092 0.766062 0.081999

H -4.580571 -1.215006 -0.193854

H -6.008176 -0.131432 -0.296593

H -4.742310 -0.059447 -1.544213

H -3.754196 1.327933 2.255506

H -5.417476 0.725674 2.018515

H -4.032996 -0.414699 1.997135

DMA·NO₃⁻·H₂O

C -4.843630 -0.350903 -0.450652

N -4.249882 0.699151 0.360009

C -4.015272 0.228747 1.720285

O -1.163421 1.100711 0.553983

N -1.140188 -0.135635 0.676427

O -0.617486 -0.659384 1.682911

O -1.657950 -0.856417 -0.209924

H -3.336219 0.923428 -0.033159

H -4.255598 -1.286974 -0.431587

H -5.857176 -0.569840 -0.080627

H -4.927931 -0.014465 -1.491924

H -3.411322 0.966238 2.260520

H -4.978969 0.113868 2.239894

H -3.488197 -0.742911 1.754198
O -1.892768 -3.213046 1.414496
H -2.054268 -2.743580 0.582675
H -1.343226 -2.534046 1.838918

DMA \cdot NO₃⁻ \cdot (H₂O)₂
C 4.785065 6.897790 7.916113
N 5.388458 5.900432 7.046028
C 5.712264 6.469265 5.744036
O 7.849805 8.285371 7.586320
N 8.709959 7.905436 6.752217
O 8.738427 8.392560 5.623302
O 9.536467 7.017428 7.088043
O 8.855784 7.388546 10.009894
O 8.062462 5.023673 8.486343
H 6.248684 5.571732 7.484546
H 5.392755 7.816281 8.002221
H 3.794381 7.174210 7.522381
H 4.642016 6.472975 8.917858
H 6.300628 5.746964 5.165048
H 4.780211 6.665086 5.190839
H 6.280488 7.413656 5.807199
H 8.587468 5.582323 7.884151
H 8.045859 5.581469 9.277514
H 9.670138 7.102367 9.578378
H 8.385590 7.778994 9.242367

DMA \cdot NO₃⁻ \cdot (H₂O)₃
C -3.169602 9.245464 8.856165
N -3.896086 10.268665 8.115082
C -3.913827 9.953402 6.692754
O -6.690133 9.210039 8.372563
O -7.719729 4.974937 7.478744
N -8.073123 5.424515 8.577730

O -7.191016 5.705058 9.446499
O -9.267741 5.611198 8.844632
O -5.408279 6.725824 7.577284
O -8.502525 8.011796 10.311546
H -4.560185 10.666630 6.167422
H -4.275851 8.929732 6.485722
H -2.896372 10.046861 6.283514
H -3.541370 8.224618 8.654222
H -2.104254 9.283161 8.582604
H -3.249335 9.444252 9.931902
H -4.864660 10.241131 8.433177
H -5.775349 6.315024 8.384650
H -5.940062 6.268886 6.912453
H -7.348412 8.902894 9.018635
H -6.286508 8.394696 8.028915
H -7.936886 7.216301 10.297846
H -9.276335 7.664249 9.849625

DMA·NO₂⁻

C -4.924838 -0.197150 -0.469761
N -4.244337 0.844236 0.281913
C -4.367740 0.600182 1.710593
O -1.255047 0.553680 0.713559
N -1.187219 -0.677698 0.922734
O -2.060776 -1.373057 0.366823
H -3.241061 0.762677 0.082073
H -4.572785 -1.209963 -0.201280
H -6.010569 -0.134413 -0.288723
H -4.751543 -0.049910 -1.543929
H -3.758363 1.329638 2.257029
H -5.419095 0.718188 2.020418
H -4.026115 -0.413239 1.994681

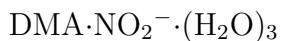
DMA·NO₂⁻·H₂O

C -4.728141 -0.564180 -0.314692
N -4.342743 0.727499 0.230044
C -4.330343 0.684491 1.684303
O -1.363522 1.373092 0.614050
N -0.982315 0.235823 0.919581
O -1.600765 -0.713648 0.370952
H -3.373593 0.903222 -0.047315
H -4.098585 -1.389802 0.064004
H -5.779246 -0.772693 -0.058740
H -4.642974 -0.543659 -1.408764
H -3.936143 1.630520 2.072800
H -5.357184 0.550747 2.060267
H -3.702522 -0.137328 2.077767
O -0.079977 -2.561780 1.687490
H 0.399479 -1.847795 2.119405
H -0.712011 -2.042470 1.135956

DMA \cdot NO₂⁻ \cdot (H₂O)₂

C -4.647784 0.469435 -0.291408
N -3.604951 0.744198 0.679719
C -4.068184 0.526815 2.042022
O -1.030268 -0.711523 2.077602
N -1.205260 -1.750365 1.425687
O -1.788493 -1.612176 0.320568
O -1.688612 -4.340664 -0.107292
H -2.834389 0.087477 0.514748
H -5.083893 -0.542739 -0.181313
H -5.461794 1.201979 -0.181760
H -4.241296 0.558109 -1.306015
H -3.228120 0.662996 2.731009
H -4.853907 1.257690 2.286717
H -4.481850 -0.488918 2.194375
H -1.814300 -3.367197 -0.136524

H -1.234486 -4.435246 0.735972
O -1.168091 2.158744 1.476864
H -0.953579 1.226514 1.654224
H -2.036072 2.070294 1.052277



N -3.007392 9.321164 8.744791
C -3.880955 10.248085 8.034759
C -2.548511 8.266751 7.852952
H -1.805144 7.645870 8.366896
H -3.398139 7.625870 7.572689
H -2.094075 8.659164 6.923984
H -3.421602 10.650034 7.113734
H -4.137807 11.086171 8.693828
H -4.814007 9.732568 7.760794
H -2.181809 9.847537 9.029183
O -0.536622 10.892880 8.318426
H 0.229454 11.492415 8.341813
H -0.833311 10.913444 7.393354
O 1.653788 12.786747 8.106958
H 1.284939 12.987234 7.219475
H 2.466944 12.341354 7.838507
O -1.379698 10.953964 5.502233
H -0.701723 11.672339 5.413547
H -0.919617 10.194977 5.128984
O 0.731419 12.589993 5.525447
N 1.578173 11.742939 5.096899
O 2.722555 11.877137 5.522500



O 10.008120 3.543256 5.215516
N 9.176319 3.836659 6.092076
O 7.966740 3.841675 5.850948
O 9.586947 4.134356 7.250960

N 7.142865 4.674356 8.601350

C 6.321348 3.450030 8.538353

C 6.525355 5.810591 7.890296

H 5.569233 6.029170 8.372254

H 6.404077 5.539927 6.837954

H 7.189180 6.675373 7.979557

H 5.364970 3.662224 9.022747

H 6.841637 2.656801 9.082938

H 6.198311 3.164810 7.490166

H 7.266870 4.945165 9.630879

H 8.066785 4.479240 8.172296

N 6.165727 5.560092 11.545454

O 5.245964 5.419209 10.713273

O 7.362785 5.349313 11.162406

O 5.947641 5.890940 12.701997

N 12.501488 3.769216 6.564786

H 11.629541 3.670954 6.012853

C 12.612268 5.165408 7.030585

H 13.350426 3.552319 5.947008

C 12.467978 2.800769 7.677952

N 15.637173 3.426222 5.883637

O 14.654838 3.279229 5.085515

O 15.394047 3.727562 7.070147

O 16.779566 3.271543 5.475409

H 12.382160 1.794488 7.258039

H 13.406263 2.890962 8.230560

H 11.599920 3.019262 8.305644

H 13.550666 5.262233 7.582034

H 12.629282 5.820905 6.155210

H 11.744633 5.396124 7.654449

DMA₂·(HNO₃)₂·NO₃⁻·H₂O

C -6.288423 11.214214 4.094861

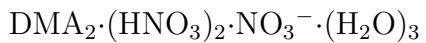
N -5.026996 11.227043 3.327904
C -4.140818 12.358894 3.659752
O -5.040032 8.446025 4.755310
N -4.394824 7.937189 3.816930
O -3.833062 6.847620 3.936549
O -4.327639 8.565735 2.723390
O -4.776175 11.375445 -1.186908
N -4.745604 11.386676 0.036277
O -5.754342 11.726879 0.706509
O -3.699184 11.063653 0.660590
N -1.876706 9.337293 1.751160
C -0.918892 10.201166 1.036435
C -1.473446 7.919187 1.825075
O -2.356860 10.063659 4.310848
N -1.477578 10.917317 4.641005
O -1.590541 11.511567 5.717330
O -0.538293 11.140086 3.864898
H -3.251166 12.290359 3.028574
H -3.877223 12.302043 4.718502
H -4.677245 13.286865 3.436744
H -6.044051 11.236487 5.160167
H -6.820072 10.291255 3.853144
H -6.877348 12.089305 3.800247
H -4.544367 10.322493 3.458668
H -5.250056 11.285471 2.308852
H -2.806683 9.430980 1.323257
H -2.018833 9.678116 2.742353
H 0.047063 10.139423 1.542764
H -0.848910 9.864593 -0.002890
H -1.291578 11.225487 1.066949
H -0.520265 7.867397 2.360549
H -2.248097 7.368627 2.367291

H -1.353664 7.527595 0.809384
 O -4.271435 10.615222 6.554714
 H -4.372564 9.794266 6.047006
 H -3.342554 10.851419 6.405508

$\text{DMA}_2\cdot(\text{HNO}_3)_2\cdot\text{NO}_3^- \cdot (\text{H}_2\text{O})_2$

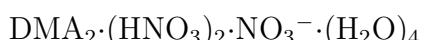
C 4.472130 9.759092 2.560529
 N 5.479441 9.422996 1.535062
 C 5.062780 8.323141 0.645321
 O 6.011325 11.276140 -0.493016
 N 4.940529 11.952437 -0.450510
 O 4.952748 13.133463 -0.813570
 O 3.906319 11.407074 -0.039724
 O 7.317499 11.919448 4.264977
 N 7.027028 12.585639 3.246877
 O 6.461168 12.017207 2.283967
 O 7.320693 13.785516 3.171567
 O 7.566278 9.259751 3.335340
 O 8.069770 8.584433 0.358712
 N 9.171043 8.133072 0.785629
 O 9.592139 7.050209 0.407245
 O 9.816766 8.839243 1.604079
 N 8.579234 11.348622 0.550674
 C 9.525552 11.844076 1.569099
 C 9.099965 11.431815 -0.826183
 H 4.152372 8.641758 0.128811
 H 4.876115 7.428386 1.247864
 H 5.867458 8.133551 -0.066595
 H 4.286808 8.866465 3.167009
 H 3.562498 10.090616 2.053732
 H 4.876399 10.564171 3.176596
 H 5.662495 10.245328 0.925482
 H 6.376863 9.218773 2.027136

H 7.715495 11.911036 0.593961
H 8.326001 10.358584 0.730821
H 9.137941 11.605120 2.562410
H 10.483779 11.338760 1.428595
H 9.612255 12.927015 1.447184
H 9.985517 10.793239 -0.900495
H 8.313857 11.085966 -1.500397
H 9.341148 12.477961 -1.033130
H 8.441405 9.187024 2.916738
H 7.501220 10.161762 3.708419
O 7.524774 13.977196 0.238960
H 6.682807 13.777304 -0.206949
H 7.281296 14.071617 1.175310



C 7.631602 6.984761 6.219120
N 6.794709 7.449595 7.345138
C 5.602394 6.609351 7.576783
O 7.589789 7.050698 10.008217
N 8.253203 5.964427 9.937236
O 8.241455 5.334526 8.870578
O 8.885002 5.579528 10.920142
O 7.203911 10.321387 6.270608
O 4.567159 9.456148 10.081638
N 5.203174 9.651988 9.033580
O 6.426245 9.936897 9.082645
O 4.646342 9.550549 7.927365
N 8.742155 9.565505 10.721500
C 9.810263 8.856839 11.451119
C 8.857427 11.033440 10.757420
O 10.875436 10.044606 8.497171
N 10.035011 9.621755 7.696516
O 9.086596 8.894914 8.113196

O 10.080889 9.901132 6.488245
O 6.441829 8.629438 12.007228
H 8.162727 10.162454 6.232684
H 6.994183 10.383048 7.218704
H 5.952573 5.600063 7.808550
H 4.988347 6.632808 6.672936
H 5.047492 7.020018 8.423755
H 8.469818 7.677572 6.116401
H 7.992415 5.983366 6.465129
H 7.008936 6.986905 5.320413
H 6.505125 8.416881 7.159017
H 7.340001 7.457500 8.227799
H 7.819078 9.279030 11.106463
H 8.770917 9.244314 9.725114
H 8.032828 11.448255 10.172369
H 8.786321 11.369879 11.797225
H 9.818887 11.317916 10.321501
H 10.762983 9.087356 10.965420
H 9.812062 9.193639 12.493362
H 9.601765 7.783242 11.403176
H 5.734976 8.981822 11.431687
H 6.679149 7.788602 11.580925
O 5.138505 8.772528 5.152475
H 5.880167 9.385189 5.308449
H 4.542528 9.007631 5.874892



C 8.016932 7.462037 9.075079
N 7.388491 8.742342 8.689182
C 6.356840 9.189904 9.655419
O 6.925661 8.314030 5.991972
O 4.208743 8.644731 6.762763
N 4.188515 7.940806 7.787287

O 4.990833 6.981610 7.891059
O 3.398295 8.199179 8.714690
O 6.621162 11.110546 7.213984
N 6.969523 11.696377 6.161054
O 7.182119 11.062686 5.127429
O 7.104389 12.946494 6.180190
N 7.363497 13.240028 8.882410
C 6.119934 13.134001 9.673777
C 8.203835 14.394778 9.240136
O 8.973820 11.026146 9.307236
N 9.038590 10.954610 10.570030
O 8.786058 11.977197 11.235307
O 9.326589 9.885180 11.105254
O 3.867515 11.098158 8.382803
H 6.997837 9.211590 5.621321
H 5.965923 8.162458 6.045775
H 6.863795 9.487149 10.578282
H 5.684506 8.355243 9.864911
H 5.803726 10.024518 9.219924
H 8.725324 7.175857 8.293557
H 8.529785 7.602308 10.030192
H 7.225261 6.713113 9.159322
H 7.014309 8.646346 7.715367
H 8.101325 9.485238 8.644392
H 7.926988 12.372420 9.019767
H 7.145331 13.239326 7.856425
H 5.562389 14.071500 9.580317
H 5.513817 12.312623 9.279962
H 6.393824 12.957451 10.717979
H 9.100417 14.380704 8.614502
H 7.640966 15.316870 9.064449
H 8.486269 14.305571 10.292403

H 3.428061 10.239930 8.494156
H 4.428186 10.940982 7.609991
O 9.675983 11.056742 13.866755
H 9.326397 11.559655 13.115883
H 9.779631 10.186902 13.465402
O 4.646737 6.201998 10.582483
H 4.768053 6.280307 9.619347
H 3.904301 6.802017 10.715226

DMA₂·(HNO₃)₂·NO₂⁻
C 2.724309 6.900274 2.576245
N 2.513033 7.686639 3.806888
C 1.101317 8.069988 4.000184
O 3.185065 6.139254 5.888323
N 2.402617 5.139226 5.809489
O 2.469024 4.246664 6.644665
O 1.581476 5.101514 4.869352
O 4.005592 10.031476 3.467595
N 3.473449 10.549638 2.440299
O 2.499656 9.990817 1.915672
O 3.937840 11.601285 1.985354
N 5.742457 12.440912 4.201641
C 6.453726 11.415901 4.969850
C 4.553011 12.915444 4.914625
O 7.330949 14.415815 3.995645
N 7.509894 14.705372 5.270732
O 8.249195 15.627571 5.448117
H 0.512023 7.153677 4.087162
H 0.789187 8.684502 3.151790
H 1.024662 8.646683 4.926572
H 2.418578 7.507804 1.720249
H 2.141802 5.979312 2.659451
H 3.788569 6.659180 2.500401

H 2.815942 7.096974 4.641036

H 3.090619 8.552233 3.746383

H 5.404987 12.026218 3.328872

H 6.644519 13.567738 4.013073

H 5.796359 10.568433 5.205798

H 7.308269 11.054927 4.387142

H 6.828464 11.865670 5.897653

H 4.865657 13.404302 5.845587

H 4.027599 13.643352 4.287864

H 3.874347 12.081319 5.143276

DMA₂·(HNO₃)₂·NO₂⁻·H₂O

C 2.776763 -6.210149 5.901377

N 1.353254 -5.872290 6.103237

C 0.764071 -5.171663 4.944206

O 0.004453 -8.208019 6.413777

N 0.200838 -8.822883 5.330121

O 0.903707 -8.267581 4.449077

O -0.285477 -9.933273 5.150025

O 1.223069 -4.098008 8.277684

N 1.920552 -3.126874 7.859337

O 2.069434 -2.133612 8.586753

O 2.437407 -3.186815 6.738978

O 0.806190 -10.311668 2.394083

N 0.591400 -2.815415 10.960706

C -0.805218 -3.069665 10.565587

C 1.247314 -4.015015 11.510286

O -0.584961 -2.636831 13.700308

N -0.143939 -1.495379 13.853121

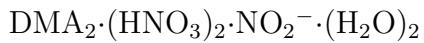
O 0.517309 -1.035227 12.873151

H 0.829619 -5.834723 4.078258

H 1.311878 -4.238484 4.790622

H -0.284815 -4.957007 5.167337

H 2.847894 -6.875146 5.037347
H 3.139402 -6.725208 6.795371
H 3.333793 -5.281575 5.753338
H 0.815637 -6.767086 6.263619
H 1.271826 -5.257621 6.940011
H 1.123124 -2.492566 10.136442
H 0.582189 -2.044370 11.748314
H 2.281431 -3.760942 11.761281
H 0.708822 -4.303187 12.417638
H 1.230227 -4.808376 10.757415
H -0.825890 -3.863055 9.812992
H -1.360255 -3.348317 11.465914
H -1.221321 -2.148116 10.147791
H 0.969730 -9.516976 2.926914
H 0.259189 -10.813992 3.008609



C 4.731702 3.240185 6.782193
N 4.073740 4.206721 5.882076
C 2.602009 4.184900 5.960489
O 5.442069 6.429594 6.695636
N 5.115130 6.567221 7.922323
O 4.078026 5.996065 8.242939
O 3.753010 5.143800 3.206312
N 2.912084 5.962014 2.700071
O 3.338967 7.040663 2.259591
O 1.724140 5.662569 2.671277
O 3.761013 2.236444 3.733403
O 6.569710 1.815839 4.385701
N 6.953292 2.982824 4.549979
O 6.287079 3.930166 4.060364
O 7.977917 3.230475 5.212236
N 6.012263 6.651280 3.616136

C 6.601158 6.486476 2.275023
C 5.746913 8.055383 3.981058
O 7.932686 6.061099 5.528572
H 2.266868 3.159235 5.782605
H 2.204432 4.835106 5.176351
H 2.315681 4.542368 6.953239
H 4.505116 2.229947 6.430922
H 4.359645 3.410579 7.796028
H 5.811202 3.417583 6.753048
H 4.449412 5.159929 6.127246
H 4.360476 3.996350 4.920335
H 5.128782 6.092471 3.609314
H 6.665797 6.242955 4.319955
H 5.059483 8.481866 3.246780
H 5.306351 8.064527 4.981019
H 6.700607 8.593576 3.993749
H 5.890720 6.878717 1.541472
H 7.550921 7.029660 2.234485
H 6.765815 5.418153 2.115934
H 4.718517 2.065743 3.741479
H 3.660631 3.051438 3.219398
H 7.247418 6.206757 6.207547
H 8.022402 5.090577 5.460371

DMA·(HNO₃)₂·NO₃⁻

C -1.109551 -0.558050 1.286808
N -1.412300 0.272685 0.101838
C -0.992549 -0.376597 -1.158741
O -4.047075 0.668993 0.116973
N -4.551514 -0.492523 -0.020151
O -3.776900 -1.461442 -0.149707
O -5.767949 -0.630088 -0.021252
O 0.449206 2.316640 -1.053381

N 1.338652 1.800527 -0.374866
O 2.488354 1.625193 -0.885861
O 1.131792 1.434376 0.790658
O 3.814403 0.046056 0.484405
N 3.174770 -1.104259 0.622296
O 2.132811 -1.260336 0.010460
H -2.466339 0.456350 0.076234
H -0.909402 1.164083 0.179509
H 0.082980 -0.574273 -1.109825
H -1.212566 0.301298 -1.986428
H -1.563967 -1.302496 -1.258027
H -1.722752 -1.460030 1.218799
H -1.372591 0.008880 2.183819
H -0.041114 -0.790600 1.287654
H 3.198740 0.704463 -0.087308
O 3.695247 -1.918197 1.349842

DMA·(HNO₃)₂·NO₃⁻·H₂O
C 0.452092 -0.297255 -1.120059
N 0.646589 0.660312 -0.010415
C 0.467502 0.023516 1.311901
O 3.196454 1.601555 -0.150866
N 3.920006 0.577440 -0.020392
O 3.358366 -0.534830 0.129820
O 5.143172 0.677659 -0.041326
O -1.337237 2.782297 -0.276518
N -2.370386 2.102414 -0.180112
O -3.490197 2.578627 -0.234240
O -2.218005 0.838194 -0.015888
O -4.256190 -0.565765 0.185680
N -3.792744 -1.799882 0.346444
O -4.624367 -2.666924 0.467869
O 5.737944 -2.200349 0.333812

H -0.545678 -0.734322 -1.028136
H 0.544966 0.244541 -2.065333
H 1.234934 -1.055857 -1.046047
H 1.250710 -0.729503 1.427424
H -0.530552 -0.420961 1.348831
H 0.571094 0.791757 2.083125
H -0.035044 1.431965 -0.107842
H 1.623891 1.054693 -0.068640
H 4.813393 -1.909316 0.301303
H 6.176457 -1.348759 0.218993
H -3.416943 0.073218 0.094610
O -2.584423 -1.959180 0.358778

DMA·(HNO₃)₂·NO₃⁻·(H₂O)₂
C 0.714071 -0.627815 -0.533455
N 0.865471 -0.227627 0.886579
C 0.020831 -1.019778 1.801565
O 2.886025 -2.512656 0.713769
N 3.623914 -1.584654 0.360958
O 4.346290 -1.655988 -0.633694
O 3.607578 -0.503047 1.043003
O 1.383651 2.442051 0.233573
O -1.034757 2.441545 -1.290090
N -1.824300 1.799661 -0.594450
O -1.502593 1.338719 0.507888
O -3.001292 1.604737 -1.029092
O -4.221324 0.001599 0.399727
N -3.585223 -1.156682 0.448412
O -4.005546 -1.964486 1.245571
O 3.730352 1.341059 -0.992366
H -0.327948 -0.473503 -0.823466
H 1.383185 -0.000660 -1.128621
H 0.993152 -1.680350 -0.623281

H -1.017633 -0.936533 1.474373
H 0.136118 -0.627095 2.815013
H 0.364297 -2.056863 1.758447
H 0.661520 0.784714 0.933570
H 1.870473 -0.328883 1.144474
H 2.130744 2.240257 -0.353657
H 0.613510 2.587397 -0.342141
H -3.650513 0.665582 -0.217367
H 3.869600 0.778687 -0.202756
H 3.969102 0.743870 -1.708825
O -2.640422 -1.325325 -0.302546

DMA·(HNO₃)₂·NO₃⁻·(H₂O)₃

C -0.235183 0.122724 0.841836
N -0.539598 -0.208922 -0.568391
C 0.025372 -1.505857 -0.992230
O -3.328979 -0.564329 -1.266990
N -3.763296 -0.880848 -0.129292
O -4.950353 -0.717810 0.156271
O -2.952901 -1.327933 0.717876
O -2.756728 2.103457 -0.233927
O -0.325113 2.331775 -1.681047
O 2.032847 2.649302 -0.116404
N 2.622220 1.577792 -0.281926
O 3.695703 1.367130 0.362333
O 2.193139 0.706621 -1.046951
O 4.543087 -0.927428 0.004823
N 3.685675 -1.834918 0.440679
O 2.702807 -1.450482 1.050185
O 3.958503 -2.988054 0.197128
H 0.848510 0.107508 0.974023
H -0.644955 1.113515 1.051150
H -0.708586 -0.629829 1.475886

H 1.108640 -1.471855 -0.863221
H -0.238332 -1.672357 -2.039618
H -0.418044 -2.285369 -0.366255
H -0.205607 0.577269 -1.161764
H -1.564345 -0.255942 -0.702622
H -1.077886 2.562628 -1.113036
H 0.478171 2.606057 -1.204440
H 4.116737 0.039904 0.167281
H -3.184110 1.464486 -0.823201
H -3.073604 1.862475 0.655181
O -3.740177 0.957617 2.211091
H -4.619230 0.739653 1.872060
H -3.280328 0.112347 2.075181

DMA·(HNO₃)₂·NO₃⁻·(H₂O)₄

C -0.597031 -1.728155 -0.174341
N 0.494690 -1.076448 0.579875
C 0.993813 -1.889272 1.708620
O 0.827617 1.421363 2.200086
O 3.311927 0.547262 1.304974
O 0.619168 2.137417 -0.561300
N -0.405243 1.568651 -0.961051
O -0.612828 1.310879 -2.133450
O -1.275272 1.227719 -0.073444
O -3.243038 0.237472 -1.241152
N -4.037809 -0.336711 -0.351690
O -5.049786 -0.832721 -0.780645
O -3.690544 -0.327550 0.819333
O 3.445132 1.901422 -1.145128
O 3.326867 -1.926207 -0.242823
N 3.260336 -1.164878 -1.236237
O 4.272035 -0.833520 -1.855896
O 2.137755 -0.706358 -1.573324

H -1.481736 -1.772821 0.467591
H -0.798259 -1.143774 -1.076019
H -0.262361 -2.730756 -0.455964
H 0.144472 -2.125850 2.353535
H 1.728099 -1.293885 2.256160
H 1.473492 -2.781025 1.299715
H 0.161125 -0.178753 0.955553
H 1.262488 -0.882446 -0.106221
H 1.746070 1.128041 2.038607
H 0.620229 1.937881 1.404712
H -2.409968 0.651035 -0.726367
H 3.530227 -0.355983 1.031548
H 3.442671 1.085239 0.494646
H 3.742071 1.170763 -1.709275
H 2.484032 1.924501 -1.276300
H -2.097710 0.078971 2.086272
O -1.409089 -0.242884 2.681699
H -0.739202 0.461644 2.700292

DMA·(HNO₃)₂·NO₂⁻
C 4.853461 8.269566 6.347350
N 3.734562 8.586205 7.256987
C 3.450796 10.033256 7.325047
O 1.530127 7.413920 6.285108
N 1.375956 7.927586 5.131588
O 2.209782 8.771188 4.741771
O 0.426328 7.589467 4.436406
O 4.607362 7.774879 9.815479
N 5.609826 8.497041 9.991381
O 6.277481 8.372192 11.042427
O 5.942805 9.330733 9.135680
O 8.360528 9.954978 11.136206
N 9.229840 9.489937 10.235535

O 10.249617 10.101261 10.241414
H 5.752295 8.772485 6.714199
H 5.004610 7.186228 6.351410
H 4.575191 8.600359 5.343590
H 3.167824 10.367422 6.323690
H 4.342618 10.545228 7.695726
H 2.616827 10.188480 8.015756
H 3.980731 8.248825 8.209061
H 2.859419 8.090205 6.904302
H 7.543902 9.372821 11.035479

DMA·(HNO₃)₂·NO₂⁻·H₂O
C 4.570781 8.078255 6.500450
N 3.543509 8.376944 7.519149
C 3.167929 9.805187 7.547188
O 1.285871 6.987902 6.863036
N 0.974914 7.426116 5.723528
O -0.022945 7.003600 5.147445
O 1.708742 8.300199 5.198715
O 0.248904 8.703569 2.723382
O 4.723915 7.747371 9.968483
N 5.694332 8.534381 10.008249
O 5.877506 9.349402 9.091311
O 6.476712 8.491659 10.980851
H 5.467476 8.656885 6.736708
H 4.795754 7.008773 6.541199
H 4.161905 8.334597 5.520117
H 2.752193 10.065614 6.570762
H 4.059494 10.390505 7.785085
H 2.410016 9.947244 8.322797
H 3.921299 8.109870 8.454489
H 2.681701 7.810165 7.305678
H -0.344466 8.030576 3.076808

H 0.894181 8.747050 3.447001
H 7.681912 9.573224 10.794666
N 9.250066 9.757877 9.795504
O 8.464601 10.203495 10.781654
O 10.223206 10.426897 9.664075
DMA.(HNO3)2.NO2-(H2O)2
C 4.618232 7.865207 6.527781
N 3.678443 8.490232 7.484708
C 3.567942 9.952985 7.298718
O 1.166345 7.513604 7.110290
N 0.898923 7.782249 5.908083
O 1.775647 8.353223 5.214873
O -0.195981 7.488410 5.437203
O 5.116415 7.222781 9.690853
N 5.871553 8.157337 9.977246
O 6.891357 7.957578 10.670948
O 5.614773 9.316333 9.570775
O 8.315796 10.103442 11.108570
N 8.652633 10.568963 9.906522
O 9.371775 11.513259 9.970233
O 0.307263 8.540603 2.711147
H 5.596639 8.343502 6.638817
H 4.682895 6.799135 6.759384
H 4.217853 8.012245 5.521961
H 3.098404 10.125940 6.327082
H 4.568108 10.391649 7.340588
H 2.942502 10.357485 8.098560
H 4.021667 8.279600 8.432246
H 2.719849 8.066176 7.361628
H -0.378063 8.103716 3.230775
H 1.000690 8.608222 3.386059
H 7.716457 9.314230 10.921409

O 6.986210 10.182267 7.272383

H 6.672361 9.942714 8.160925

H 7.882665 10.490779 7.436609

- [1] J. Lengyel, M. Ončák, J. Fedor, J. Kočíšek, A. Pysanenko, M. K. Beyer, and M. Fárník, Electron-triggered chemistry in hno₃/h₂o complexes, Phys. Chem. Chem. Phys. **19**, 11753 (2017).
- [2] J. Lengyel, J. Fedor, and M. Fárník, Dissociative electron attachment to hno₃ and its hydrates:energy-selective electron-induced chemistry, Phys. Chem. Chem. Phys. **21**, 8691 (2019).
- [3] J. Lengyel, J. Kočíšek, M. Fárník, and J. Fedor, Self-scavenging of electrons in fe(co)₅ aggregates deposited on argon nanoparticles, J. Phys. Chem. C **120**, 7397 (2016).