Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Thermochemistry and Crystal Structure Predictions of Energetic Derivatives of Formamidine Salts

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Contents:

S1. The structures of ionic and neutral parts for calculations.

Nitrate anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.000000
2	8	0	0.000000	1.262676	0.000000
3	8	0	1.093509	-0.631338	0.000000
4	8	0	-1.093509	-0.631338	0.000000

Nitric acid

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.153278	0.000000
2	8	0	-0.988520	0.833436	0.000000
3	8	0	1.172698	0.469945	0.000000
4	8	0	-0.262521	-1.233511	0.000000
5	1	0	0.626743	-1.631907	0.000000

Dinitramide anion

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.800391
2	7	0	0.000000	1.158837	0.056489
3	8	0	-0.481988	1.236388	-1.080810
4	8	0	0.421228	2.150544	0.681211
5	7	0	0.000000	-1.158837	0.056489
6	8	0	0.481988	-1.236388	-1.080810
7	8	0	-0.421228	-2.150544	0.681211

Dinitramic acid

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	7	0	-0.604522	-0.450746	0.000000
2	7	0	-0.016175	0.005130	1.253173
3	8	0	0.330495	1.154191	1.343066
4	8	0	-0.016175	-0.869483	2.102427
5	7	0	-0.016175	0.005130	-1.253173
6	8	0	0.330495	1.154191	-1.343066
7	8	0	-0.016175	-0.869483	-2.102427
8	1	0	-0.571005	-1.471919	0.000000

Formamidinium

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.431146
2	7	0	0.000000	1.166204	-0.176628
3	1	0	0.000000	2.019680	0.369738
4	1	0	0.000000	1.259574	-1.187843
5	7	0	0.000000	-1.166204	-0.176628
6	1	0	0.000000	-2.019680	0.369738
7	1	0	0.000000	-1.259574	-1.187843
8	1	0	0.000000	0.000000	1.522120

Formamidine

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.122435	0.393479	-0.000665
2	7	0	1.136898	-0.149274	-0.052296
3	1	0	1.928457	0.419474	0.205718
4	1	0	1.215993	-1.148178	0.091888
5	7	0	-1.176983	-0.333503	0.010956
6	1	0	-2.011098	0.251991	0.001580
7	1	0	-0.118144	1.495281	-0.005810

Azidoformamidinium

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.796514	0.000000

2	7	0	1.333003	0.759724	0.000000
3	1	0	1.844854	-0.113091	0.000000
4	1	0	1.880363	1.611806	0.000000
5	7	0	-0.665918	1.945287	0.000000
6	1	0	-1.679492	1.932800	0.000000
7	1	0	-0.193967	2.840170	0.000000
8	7	0	-0.801495	-0.316891	0.000000
9	7	0	-0.234084	-1.446143	0.000000
10	7	0	0.103957	-2.520658	0.000000

Azidoformamidine

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.803691	0.118371	-0.002230
2	7	0	0.615983	1.384486	0.007064
3	1	0	1.497166	1.898022	-0.001505
4	7	0	1.986743	-0.587312	-0.059398
5	7	0	-0.291887	-0.795183	0.002516
6	7	0	-1.414234	-0.253468	0.000710
7	7	0	-2.484407	0.115862	0.001098
8	1	0	2.832773	-0.089207	0.173631
9	1	0	1.962532	-1.569733	0.177327

Guanidinium

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	7	0	0.000000	1.337339	0.000000
3	1	0	0.863621	1.862160	0.000000
4	1	0	-0.863621	1.862160	0.000000
5	7	0	1.158170	-0.668670	0.000000
6	1	0	1.180867	-1.678998	0.000000
7	1	0	2.044488	-0.183162	0.000000
8	7	0	-1.158170	-0.668670	0.000000
9	1	0	-2.044488	-0.183162	0.000000
10	1	0	-1.180867	-1.678998	0.000000

Guanidine

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.019120	0.121110	0.000133
2	7	0	-0.249331	1.384940	0.009745
3	1	0	-1.249227	1.580829	-0.045764
4	7	0	1.288485	-0.355572	-0.081501
5	1	0	1.487459	-1.161726	0.499901
6	1	0	1.971160	0.386062	0.020746
7	7	0	-0.959340	-0.912031	0.076164
8	1	0	-1.918586	-0.613466	-0.042023
9	1	0	-0.734782	-1.739720	-0.464516

Nitroformamidinium

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.699560
2	7	0	0.000000	1.181150	-1.252934
3	1	0	0.000000	1.996012	-0.638406
4	1	0	0.000000	1.315732	-2.259871
5	7	0	0.000000	-1.181150	-1.252934
6	1	0	0.000000	-1.315732	-2.259871
7	1	0	0.000000	-1.996012	-0.638406
8	7	0	0.000000	0.000000	0.836618
9	8	0	0.000000	-1.096963	1.354917
10	8	0	0.000000	1.096963	1.354917

Nitroformamidine

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.774340	0.000000
2	7	0	-1.023903	1.512048	0.000000
3	7	0	1.297598	1.149538	0.000000
4	1	0	1.510979	2.134850	0.000000
5	1	0	2.028290	0.454743	0.000000
6	7	0	-0.123659	-0.780798	0.000000
7	8	0	0.914480	-1.433053	0.000000
8	8	0	-1.252973	-1.236933	0.000000
9	1	0	-1.881580	0.958743	0.000000

S2. Lattice energy minimization.

The optimal geometry and distributions of electrostatic potentials of the molecules and ions were calculated on the program package Gaussian 09 using DFT method with B3LYP functional and the extended basis aug-cc-PVDZ. Grimme dispersion correction (version 2) was used (GD2). The optimized molecular structures were treated as rigid bodies throughout the lattice energy calculations in this study.

The current version of program PMC was used throughout the crystal packing calculations. In calculation of lattice energy the convergence acceleration was applied for both the r-1 electrostatic and r- 6 dispersion terms in the lattice sums with the convergence Kconv of 0.175 and the cutoff parameters Rcut=9 A and R*=0.5 A for direct and reciprocal spaces, respectively. During minimization, the parameters of the unit cell and six parameters of rigid body of the crystallographically independent molecules were varied simultaneously, including three components of the center of mass and three Euler angles, while all the other molecules in the crystal environment perform the dependent motion in accordance with the symmetry group of a crystal. The local energy minimization was performed with the quasi Newton method using the Fortran subroutine VA09 A with analytical first derivatives. Each local minimum was refined in a series of few minimization stages: at each stage (p), lists of pairs of atoms {i, j} and points of the reciprocal space {h, k, l} contributing to the approximate energy function of the lattice F(p) are not updated to ensure continuity and perfect integrity F(p) with smooth motion from the initial X0(p) to the lower point of Xmin(p); at which these lists are updated and the next minimization stage, p+1, is carried out starting from X0(p+1)=Xmin(p) down to a new minimum approximation Xmin (p+1), and etc., until the self-consistency condition Xmin (s)=Xmin (s- 1) is finally reached.

The enthalpies (H) and free energies (G) were calculated using the complete basis set (CBS) method of Petersson and coworkers in order to obtain very accurate energies. The CBS models use the known asymptotic convergence of pair natural orbital expressions to extrapolate from calculations using a finite basis set to the estimated complete basis set limit. CBS-4 begins with a HF/3-21G(d) geometry optimization; the zero point energy is computed at the same level. It then uses a large basis set SCF calculation as a base energy, and a MP2/6-31+G calculation with a CBS extrapolation to correct the energy through second order. A MP4(SDQ)/6-31+(d,p) calculation is used to approximate higher order contributions. In this study we applied the modified CBS-4M method (M referring to the use of Minimal Population localization) which is a re-parametrized version of the original CBS-4 method and also includes some additional empirical corrections. In addition, we applied G3B3 methods.

The enthalpies of the gas-phase species M were computed according to the atomization energy method:

$$\Delta H_f°(g, M, 298) = H(Molecule, 298) - \Sigma H°(Atoms, 298) + \Sigma \Delta H_f°(Atoms, 298)$$

Table **S3.** Literature values for atomic H° and $\Delta H_f°$ (kcal mol^{-1}).

	H°(Atoms, 298)	$\Delta H_f°$(Atoms, 298) CBS-4M	$\Delta H_f°$(Atoms, 298) G3B3
H	52.1	-0.50099	-0.49872823
C	171.3	-37.7862	-37.8259642
N	113	-54.5225	-54.56280323
O	59.6	-74.9912	-75.02973288

Table **S4**. Fitting coefficients for VBT method for salts MpXq (q:p).

Anion:Cation	α, kcal mol^{-1}nm^{-1}	β, kcal mol^{-1}
1:1	117.3	51.9
2:1	133.5	60.9
1:2	165.3	-29.8
2:2	101.6	91.5

Table **S5.** Atom-atom potentials LJ 6-12.

Atom 1	Atom 2	r, A	E, kcal mol^{-1}
H	H	2.930	-0.0359
H	C	3.315	-0.0474
H	N	3.460	-0.0357
H	O	3.025	-0.0795
H	N'	3.460	-0.0357
H	H*	2.805	-0.0467
C	C	3.700	-0.0722
C	N	3.845	-0.0567
C	O	3.410	-0.1170
C	N'	3.845	-0.0567
C	H*	3.190	-0.0597
N	N	3.990	-0.0450
N	O	3.555	-0.0906
N	N'	3.990	-0.0450
N	H*	3.335	-0.0445
O	O	3.120	-0.2001
O	N'	3.555	-0.0906
O	H*	1.900	-1.1100
N'	N'	3.990	-0.0450
N'	H*	1.960	-0.9000
H*	H*	2.680	-0.0614

N' - N(sp2); H* - H which form hydrogen-bonds.

S6. Optimized crystal structure coordinates for formamidinium nitrate (ionic form).

```
data_HF_NO3_1
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.72053E+02 E(coul)=-1.60016E+02 E(vdW)=-1.20365E+01 Density= 1.78340
;
_cell_length_a    4.937
_cell_length_b    9.395
_cell_length_c    7.241
_cell_angle_alpha    97.37
_cell_angle_beta    106.79
_cell_angle_gamma    38.93
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loop_
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_atom_site_fract_y
_atom_site_fract_z
C1       -0.05680   0.71206   0.68877                                  #  1
N2       -0.05176   0.85111   0.71922                                  #  2
H*3       -0.00856   0.89121   0.61669                                  #  3
H*4       -0.08974   0.92213   0.84288                                  #  4
N5       -0.11030   0.64864   0.81139                                  #  5
H*6       -0.10994   0.54055   0.77631                                  #  6
H*7       -0.15297   0.70345   0.94243                                  #  7
H8       -0.01329   0.64419   0.55138                                  #  8
#XC1       -0.05779   0.71362   0.69191                                   #  9
#XN2       -0.04872   0.85119   0.71113                                   # 10
#XH*3       0.00285   0.90760   0.59145                                   # 11
#XH*4      -0.09499   0.93618   0.86130                                   # 12
#XN5       -0.10918   0.64206   0.80632                                   # 13
#XH*6      -0.11215   0.50983   0.77251                                   # 14
#XH*7      -0.16055   0.70941   0.96452                                   # 15
#XH8       -0.01662   0.64937   0.56187                                   # 16
N1+       0.94148   0.20080  -0.24043                                  # 17
O2+       0.96000   0.32886  -0.21688                                  # 18
O3+       0.78681   0.19546  -0.40992                                  # 19
O4+       1.07763   0.07809  -0.09448                                  # 20
#END

data_HF_NO3_2
_chemical_name_systematic
;RAS NNO22_C2_PVDZ
```

```
E(total)=-1.71796E+02 E(coul)=-1.61374E+02 E(vdW)=-1.04224E+01 Density= 1.68628
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  4 x,1/2-y,1/2+z
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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.79508   0.41250   0.37700                                  #  1
N2        0.85147   0.26876   0.39838                                  #  2
H*3       0.96671   0.25051   0.45125                                   #  3
H*4       0.78416   0.17282   0.36394                                   #  4
N5        0.64798   0.44962   0.30997                                  #  5
H*6       0.61428   0.56372   0.29814                                   #  6
H*7       0.56436   0.36815   0.26845                                   #  7
H8        0.87650   0.50820   0.41798                                  #  8
#XC1       0.79322   0.41031   0.37607                                    #  9
#XN2       0.85872   0.27038   0.40180                                    # 10
#XH*3      0.99899   0.23958   0.46587                                     # 11
#XH*4      0.77621   0.15510   0.35966                                     # 12
#XN5       0.64853   0.45717   0.31048                                    # 13
#XH*6      0.59921   0.59487   0.29219                                     # 14
#XH*7      0.54830   0.35765   0.26064                                     # 15
#XH8       0.87028   0.50089   0.41485                                    # 16
N1+       0.27694   0.15154   0.62725                                   # 17
O2+       0.41737   0.23302   0.64249                                   # 18
O3+       0.25060   0.01709   0.70421                                   # 19
O4+       0.16284   0.20452   0.53505                                   # 20
#END

data_HF_NO3_3
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.71775E+02 E(coul)=-1.60456E+02 E(vdW)=-1.13191E+01 Density= 1.72377
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_cell_length_b   11.746
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  3 -x,-y,-z
  4 1/2+x,1/2-y,z
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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.38251  -0.35308   1.02067                    #  1
N2        0.30735  -0.31580   0.80611                    #  2
H*3       0.36878  -0.24635   0.72405                    #  3
H*4       0.18825  -0.35377   0.71612                    #  4
N5        0.31486  -0.44208   1.14329                    #  5
H*6       0.38180  -0.46504   1.30800                    #  6
H*7       0.19636  -0.49016   1.08030                    #  7
H8        0.51067  -0.30667   1.10318                    #  8
#XC1       0.37957  -0.35415   1.01878                    #  9
#XN2       0.31336  -0.31150   0.80452                    # 10
#XH*3      0.38145  -0.22675   0.69354                    # 11
#XH*4      0.16920  -0.35809   0.69723                    # 12
#XN5       0.32113  -0.44193   1.15278                    # 13
#XH*6      0.39622  -0.47483   1.35594                    # 14
#XH*7      0.17762  -0.49952   1.07487                    # 15
#XH8       0.50089  -0.31022   1.09688                    # 16
N1+       0.34540   0.90108   0.36106                    # 17
O2+       0.17732   0.94330   0.42385                    # 18
O3+       0.39644   0.90194   0.13413                    # 19
O4+       0.46244   0.85800   0.52519                    # 20
#END
```

S7. Optimized crystal structure coordinates for azidoformamidinium nitrate (ionic form).

```
data_N3F_NO3_1
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.68167E+02 E(coul)=-1.58152E+02 E(vdW)=-1.00151E+01 Density= 1.64386
;
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_cell_length_b    9.527
_cell_length_c    6.377
_cell_angle_alpha    90.00
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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.52616   0.25211   0.09699                                  #  1
N2        0.61749   0.35530   0.17513                                  #  2
H*3       0.68035   0.36814   0.34788                                   #  3
H*4       0.62692   0.42473   0.06307                                   #  4
N5        0.44395   0.23582  -0.12995                                  #  5
H*6       0.37582   0.15609  -0.18264                                   #  6
H*7       0.44691   0.30068  -0.25320                                   #  7
N'8       0.50800   0.15463   0.23877                                  #  8
N9        0.58291   0.16381   0.45714                                  #  9
N'10      0.64054   0.15675   0.65402                                   # 10
#XC1       0.52348   0.25410   0.08441                                    # 11
#XN2       0.61818   0.35096   0.18620                                    # 12
#XH*3      0.70426   0.38210   0.39502                                     # 13
#XH*4      0.63285   0.44498   0.04046                                     # 14
#XN5       0.44410   0.23720  -0.13230                                    # 15
#XH*6      0.35530   0.13947  -0.21360                                     # 16
#XH*7      0.44014   0.31127  -0.29625                                     # 17
#XN'8      0.50831   0.14821   0.25286                                    # 18
#XN9       0.58500   0.15703   0.47761                                    # 19
#XN'10     0.64636   0.16935   0.64668                                     # 20
N1+       0.17077  -0.03525   0.67467                                    # 21
O2+       0.11443  -0.13723   0.53924                                    # 22
O3+       0.24410   0.04896   0.62878                                    # 23
O4+       0.15379  -0.01747   0.85598                                    # 24
#END

data_N3F_NO3_2
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.67877E+02 E(coul)=-1.57774E+02 E(vdW)=-1.01034E+01 Density= 1.67508
;
_cell_length_a   10.737
_cell_length_b    9.907
_cell_length_c    6.351
_cell_angle_alpha    90.00
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_cell_angle_gamma    90.00
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  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        -0.24404  -0.03546   0.12461                                  #  1
N2        -0.13689  -0.12440   0.02954                                  #  2
H*3       -0.12229  -0.18745  -0.10614                                   #  3
H*4       -0.06608  -0.13174   0.09067                                   #  4
N5        -0.26263   0.04702   0.30266                                  #  5
H*6       -0.34536   0.11329   0.37027                                   #  6
H*7       -0.19663   0.04609   0.37387                                   #  7
N'8       -0.34358  -0.02019   0.05061                                  #  8
N9        -0.33239  -0.09553  -0.11848                                   #  9
N'10      -0.33814  -0.15393  -0.26562                                   # 10
#XC1       -0.24208  -0.03268   0.13347                                    # 11
#XN2       -0.14128  -0.12524   0.02263                                    # 12
#XH*3      -0.10750  -0.21115  -0.14679                                     # 13
#XH*4      -0.04536  -0.13709   0.10085                                     # 14
#XN5       -0.26123   0.04692   0.30397                                   # 15
#XH*6      -0.36276   0.13348   0.39955                                     # 16
#XH*7      -0.18604   0.05325   0.40292                                     # 17
#XN'8      -0.35009  -0.02070   0.04212                                   # 18
#XN9       -0.33923  -0.09785  -0.13169                                    # 19
#XN'10     -0.32519  -0.15941  -0.26441                                     # 20
N1+        0.45886   0.32798   0.58497                                   # 21
O2+        0.54465   0.25249   0.41449                                   # 22
O3+        0.37211   0.40183   0.55743                                   # 23
O4+        0.45981   0.32962   0.78298                                   # 24
#END

data_N3F_NO3_3
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.67244E+02 E(coul)=-1.56477E+02 E(vdW)=-1.07670E+01 Density= 1.71976
;
_cell_length_a   14.369
_cell_length_b    6.373
_cell_length_c    6.257
_cell_angle_alpha    90.00
```

```
_cell_angle_beta     93.25
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        -0.61620   0.44322  -0.25004                                  #  1
N2        -0.61703   0.41652  -0.46151                                  #  2
H*3       -0.64311   0.28526  -0.53350                                   #  3
H*4       -0.59135   0.52775  -0.55766                                   #  4
N5        -0.58188   0.61585  -0.15653                                  #  5
H*6       -0.58246   0.63045   0.00470                                   #  6
H*7       -0.55493   0.73433  -0.24115                                   #  7
N'8       -0.64977   0.29927  -0.11069                                  #  8
N9        -0.68353   0.13098  -0.18875                                  #  9
N'10      -0.71569  -0.02589  -0.23094                                   # 10
#XC1       -0.61397   0.45377  -0.25018                                   # 11
#XN2       -0.61928   0.40638  -0.45665                                   # 12
#XH*3      -0.64905   0.25295  -0.57236                                    # 13
#XH*4      -0.58547   0.55228  -0.58851                                    # 14
#XN5       -0.58135   0.61816  -0.15840                                   # 15
#XH*6      -0.57940   0.64918   0.04391                                    # 16
#XH*7      -0.54688   0.77166  -0.24854                                    # 17
#XN'8      -0.65274   0.28606  -0.10286                                   # 18
#XN9       -0.68755   0.11265  -0.18203                                   # 19
#XN'10     -0.71311  -0.01590  -0.25204                                    # 20
N1+       -0.41991   0.06146   0.71494                                   # 21
O2+       -0.34827  -0.04299   0.67503                                   # 22
O3+       -0.41457   0.25808   0.73739                                   # 23
O4+       -0.49690  -0.03070   0.73241                                   # 24
#END

data_N3F_NO3_4
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.66770E+02 E(coul)=-1.57314E+02 E(vdW)=-9.45683E+00 Density= 1.63920
;
_cell_length_a    6.340
_cell_length_b    6.261
_cell_length_c    7.884
_cell_angle_alpha    92.70
```

```
_cell_angle_beta     73.79
_cell_angle_gamma    89.03
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.36156  -0.24549   0.72495                                  #  1
N2         0.33938  -0.03335   0.72467                                  #  2
H*3        0.19200   0.04419   0.77379                                   #  3
H*4        0.47052   0.05772   0.67485                                   #  4
N5         0.55545  -0.34630   0.66028                                  #  5
H*6        0.56576  -0.50779   0.66281                                   #  6
H*7        0.69442  -0.26705   0.60814                                   #  7
N'8        0.19125  -0.37823   0.79020                                  #  8
N9         0.00172  -0.29302   0.85392                                  #  9
N'10      -0.17617  -0.24409   0.91491                                   # 10
#XC1        0.37363  -0.24581   0.72069                                   # 11
#XN2        0.32758  -0.03776   0.72901                                   # 12
#XH*3       0.15655   0.08437   0.78478                                   # 13
#XH*4       0.49983   0.08744   0.66336                                   # 14
#XN5        0.55816  -0.34454   0.65926                                   # 15
#XH*6       0.58564  -0.54773   0.65731                                   # 16
#XH*7       0.73745  -0.26131   0.59272                                   # 17
#XN'8       0.17582  -0.38548   0.79593                                   # 18
#XN9       -0.01954  -0.29893   0.86166                                   # 19
#XN'10     -0.16390  -0.22348   0.90979                                   # 20
N1+        0.11041   0.78009   0.35241                                   # 21
O2+        0.31170   0.76464   0.34480                                   # 22
O3+        0.05331   0.80932   0.21390                                   # 23
O4+       -0.03377   0.76632   0.49852                                   # 24
#END

data_N3F_NO3_5
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.66698E+02 E(coul)=-1.57495E+02 E(vdW)=-9.20327E+00 Density= 1.56672
;
_cell_length_a    7.181
_cell_length_b    6.267
_cell_length_c    8.067
_cell_angle_alpha   105.82
_cell_angle_beta     86.67
_cell_angle_gamma   115.72
```

```
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.29146  -0.06197   0.27164                                  #  1
N2        0.26897  -0.12539   0.09968                                  #  2
H*3       0.20150  -0.30360   0.02872                                   #  3
H*4       0.31916   0.00394   0.03404                                   #  4
N5        0.38015   0.17225   0.36403                                  #  5
H*6       0.39447   0.21323   0.49456                                   #  6
H*7       0.43439   0.31246   0.30836                                   #  7
N'8       0.22718  -0.22729   0.36853                                  #  8
N9        0.14131  -0.45381   0.28894                                  #  9
N'10      0.06262  -0.66075   0.23922                                   # 10
#XC1       0.29662  -0.04847   0.27260                                    # 11
#XN2       0.26422  -0.13773   0.10255                                    # 12
#XH*3      0.18395  -0.35039  -0.00566                                     # 13
#XH*4      0.32980   0.03113   0.01185                                    # 14
#XN5       0.38119   0.17495   0.36277                                   # 15
#XH*6      0.40538   0.24264   0.52784                                    # 16
#XH*7      0.45234   0.35931   0.30624                                    # 17
#XN'8      0.22106  -0.24314   0.37345                                   # 18
#XN9       0.13263  -0.47639   0.29245                                    # 19
#XN'10     0.06657  -0.65086   0.22335                                    # 20
N1+       0.68393  -0.33800   0.16463                                   # 21
O2+       0.66049  -0.20298   0.08467                                   # 22
O3+       0.81351  -0.42514   0.11786                                   # 23
O4+       0.57781  -0.38587   0.29135                                   # 24
#END
```

S8. Optimized crystal structure coordinates for guanidinium nitrate (ionic form).

```
data_GH_NO3_1
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.81912E+02 E(coul)=-1.68905E+02 E(vdW)=-1.30072E+01 Density= 1.85121
;
_cell_length_a    3.448
_cell_length_b   13.231
_cell_length_c    7.312
_cell_angle_alpha    90.54
_cell_angle_beta    123.75
_cell_angle_gamma    39.73
```

```
_cell_formula_units_Z  1
_symmetry_space_group_name_H-M 'P 1     '
_symmetry_Int_Tables_number   1
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.43668   0.16474   0.53575                                  #  1
N2       -0.38756   0.37149   0.21744                                  #  2
H*3       -0.79190   0.51692   0.15112                                  #  3
H*4       -0.63015   0.38833   0.03394                                  #  4
N5        0.74035   0.14759   0.77347                                  #  5
H*6        1.36092  -0.00691   1.01548                                  #  6
H*7        0.35812   0.28863   0.71804                                  #  7
N8        0.95726  -0.02485   0.61633                                  #  8
H*9        0.74102  -0.01578   0.44064                                  #  9
H*10       1.58208  -0.18274   0.85526                                  # 10
#XN2       -0.38066   0.36976   0.22011                                 # 11
#XH*3      -0.79103   0.51484   0.14765                                  # 12
#XH*4      -0.63614   0.39170   0.03543                                  # 13
#XN5        0.73781   0.14774   0.77148                                 # 14
#XH*6       1.34063  -0.00071   1.00992                                  # 15
#XH*7       0.38029   0.28232   0.72507                                  # 16
#XN8        0.95290  -0.02326   0.61565                                 # 17
#XH*9       0.76044  -0.01990   0.44967                                  # 18
#XH*10      1.56589  -0.17979   0.84673                                  # 19
#XLP2+     -0.59338   0.39752   0.18886                                  # 20
#XLP2-     -0.14942   0.33736   0.25850                                  # 21
#XLP5+      0.51242   0.17801   0.73399                                  # 22
#XLP5-      0.95638   0.11785   0.80363                                  # 23
#XLP8+      0.72507   0.00895   0.57993                                  # 24
#XLP8-      1.16903  -0.05122   0.64957                                  # 25
N1+       0.50765   0.63100   0.46291                                  # 26
O2+       1.24952   0.44033   0.75688                                  # 27
O3+       0.20918   0.64966   0.23586                                  # 28
O4+       0.06424   0.80303   0.39597                                  # 29
#END

data_GH_NO3_2
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.77267E+02 E(coul)=-1.64586E+02 E(vdW)=-1.26811E+01 Density= 1.59517
;
_cell_length_a   12.204
_cell_length_b    7.067
_cell_length_c   13.395
_cell_angle_alpha    90.00
```

```
_cell_angle_beta    118.33
_cell_angle_gamma    90.00
_cell_formula_units_Z  8
_symmetry_space_group_name_H-M 'C 2/C   '
_symmetry_Int_Tables_number  15
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,y,1/2-z
  3 -x,-y,-z
  4 x,-y,1/2+z
  5 1/2+x,1/2+y,z
  6 1/2-x,1/2+y,1/2-z
  7 1/2-x,1/2-y,-z
  8 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.31243   0.13702  -0.12506                                  #  1
N2         0.25782   0.30092  -0.12474                                  #  2
H*3        0.17583   0.30417  -0.12324                                   #  3
H*4        0.29695   0.42633  -0.12600                                   #  4
N5         0.25852  -0.02685  -0.12337                                  #  5
H*6        0.29818  -0.15228  -0.12357                                   #  6
H*7        0.17655  -0.03003  -0.12184                                   #  7
N8         0.42094   0.13698  -0.12707                                  #  8
H*9        0.46327   0.25917  -0.12837                                   #  9
H*10       0.46379   0.01476  -0.12734                                   # 10
#XN2       0.25828   0.29955  -0.12474                                   # 11
#XH*3      0.17823   0.30726  -0.12330                                    # 12
#XH*4      0.29421   0.42425  -0.12594                                    # 13
#XN5       0.25897  -0.02547  -0.12338                                   # 14
#XH*6      0.29544  -0.15020  -0.12353                                    # 15
#XH*7      0.17895  -0.03313  -0.12187                                    # 16
#XN8       0.42003   0.13698  -0.12705                                   # 17
#XH*9      0.46361   0.25400  -0.12835                                    # 18
#XH*10     0.46411   0.01993  -0.12737                                    # 19
#XLP2+     0.24270   0.29736  -0.15484                                    # 20
#XLP2-     0.27508   0.29806  -0.09466                                    # 21
#XLP5+     0.24339  -0.02399  -0.15349                                    # 22
#XLP5-     0.27577  -0.02328  -0.09331                                    # 23
#XLP8+     0.40263   0.13663  -0.15712                                    # 24
#XLP8-     0.43500   0.13733  -0.09694                                    # 25
N1+        0.52137   0.36295   0.12500                                   # 26
O2+        0.62567   0.36291   0.12664                                   # 27
O3+        0.46919   0.20823   0.12417                                   # 28
O4+        0.46925   0.51771   0.12421                                   # 29
#END

data_GH_NO3_3
```

```
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.77264E+02 E(coul)=-1.64623E+02 E(vdW)=-1.26408E+01 Density= 1.59375
;
_cell_length_a    6.989
_cell_length_b   12.249
_cell_length_c    7.041
_cell_angle_alpha    90.00
_cell_angle_beta    122.41
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.75024   0.87039   0.24986                                  #  1
N2        0.75041   0.76121   0.24993                                  #  2
H*3       0.75309   0.71838   0.12870                                   #  3
H*4       0.74788   0.71836   0.37122                                   #  4
N5        0.75364   0.92499   0.08721                                  #  5
H*6       0.75358   1.00747   0.08397                                   #  6
H*7       0.75638   0.88536  -0.03721                                   #  7
N8        0.74665   0.92496   0.41244                                  #  8
H*9       0.74404   0.88532   0.53691                                   #  9
H*10      0.74645   1.00744   0.41557                                    # 10
#XN2       0.75041   0.76213   0.24993                                    # 11
#XH*3      0.75298   0.71804   0.13384                                    # 12
#XH*4      0.74799   0.71802   0.36609                                    # 13
#XN5       0.75362   0.92453   0.08857                                   # 14
#XH*6      0.75365   1.00505   0.08090                                    # 15
#XH*7      0.75633   0.88812  -0.03515                                    # 16
#XN8       0.74668   0.92451   0.41108                                   # 17
#XH*9      0.74408   0.88807   0.53484                                    # 18
#XH*10     0.74639   1.00503   0.41864                                    # 19
#XLP2+     0.69028   0.76333   0.21704                                    # 20
#XLP2-     0.81054   0.76338   0.28282                                    # 21
#XLP5+     0.69345   0.92390   0.05751                                    # 22
#XLP5-     0.81370   0.92394   0.12329                                    # 23
#XLP8+     0.68660   0.92387   0.37636                                    # 24
#XLP8-     0.80685   0.92392   0.44214                                    # 25
N1+       0.25026  -0.20297   0.74987                                   # 26
O2+       0.25023  -0.30605   0.74987                                   # 27
```

```
O3+       0.24809  -0.15144   0.59341                                  # 28
O4+       0.25245  -0.15143   0.90634                                  # 29
#END
```

S9. Optimized crystal structure coordinates for nitroformamidinium nitrate (ionic form).

```
data_NO2F_NO3_1
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.78243E+02 E(coul)=-1.65559E+02 E(vdW)=-1.26842E+01 Density= 1.79816
;
_cell_length_a   10.935
_cell_length_b    9.860
_cell_length_c    5.991
_cell_angle_alpha    90.00
_cell_angle_beta    119.56
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       -0.04434   0.25756   0.36471                                 #  1
N2        0.04444   0.21950   0.59833                                 #  2
H*3       0.10465   0.13590   0.62166                                  #  3
H*4       0.05554   0.26950   0.75555                                  #  4
N5       -0.13196   0.35932   0.28421                                 #  5
H*6       -0.14096   0.42524   0.40564                                  #  6
H*7       -0.19346   0.37217   0.09083                                  #  7
N8       -0.04594   0.16913   0.15216                                 #  8
O9       -0.12840   0.20422  -0.06542                                 #  9
O10       0.03544   0.07437   0.22631                                 # 10
#XC1      -0.04434   0.25760   0.36481                                  # 11
#XN2       0.04686   0.20924   0.58312                                  # 12
#XH*3      0.12802   0.12346   0.67748                                   # 13
#XH*4      0.05781   0.27647   0.78010                                   # 14
#XN5      -0.13468   0.35312   0.25985                                  # 15
#XH*6      -0.14292   0.43557   0.42265                                   # 16
#XH*7      -0.21661   0.39660   0.06381                                   # 17
#XN8      -0.04586   0.17342   0.16248                                  # 18
#XO9      -0.11987   0.18778  -0.07286                                  # 19
#XO10       0.02657   0.07172   0.18790                                   # 20
```

```
N1+       0.67945   0.05669   0.20627                                  # 21
O2+       0.62704   0.15690   0.05759                                  # 22
O3+       0.64582   0.03337   0.37623                                  # 23
O4+       0.76548  -0.02020   0.18498                                  # 24
#END

data_NO2F_NO3_2
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.78015E+02 E(coul)=-1.62878E+02 E(vdW)=-1.51373E+01 Density= 1.92897
;
_cell_length_a    6.422
_cell_length_b    6.160
_cell_length_c   13.358
_cell_angle_alpha    90.00
_cell_angle_beta     82.36
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.21544  -0.55749   0.63074                                 #  1
N2        0.31727  -0.38035   0.60168                                 #  2
H*3       0.47442  -0.37521   0.60664                                  #  3
H*4       0.24653  -0.24926   0.57468                                  #  4
N5        0.01708  -0.60459   0.63202                                 #  5
H*6      -0.08786  -0.49905   0.60848                                  #  6
H*7      -0.03287  -0.75415   0.65790                                  #  7
N8        0.34945  -0.73799   0.66929                                 #  8
O9        0.25526  -0.90302   0.69638                                 #  9
O10       0.53406  -0.69477   0.66821                                  # 10
#XC1       0.21538  -0.55740   0.63072                                  # 11
#XN2       0.33411  -0.39389   0.60483                                  # 12
#XH*3      0.50492  -0.33341   0.60003                                   # 13
#XH*4      0.23703  -0.22892   0.57055                                   # 14
#XN5       0.02518  -0.62466   0.63605                                  # 15
#XH*6     -0.10457  -0.48409   0.60507                                   # 16
#XH*7     -0.08153  -0.77149   0.65929                                   # 17
#XN8       0.34294  -0.72923   0.66742                                  # 18
#XO9       0.28452  -0.91144   0.69905                                  # 19
#XO10      0.53371  -0.72530   0.67386                                   # 20
```

```
N1+       0.21968   0.09030  -0.58041                                  # 21
O2+       0.16159   0.00607  -0.65831                                  # 22
O3+       0.25927   0.29095  -0.57863                                  # 23
O4+       0.23819  -0.02611  -0.50429                                  # 24
#END

data_NO2F_NO3_3
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.77897E+02 E(coul)=-1.63086E+02 E(vdW)=-1.48108E+01 Density= 1.92875
;
_cell_length_a    8.912
_cell_length_b   13.176
_cell_length_c    6.190
_cell_angle_alpha    90.00
_cell_angle_beta    133.89
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.25371   0.36921   0.80934                                 #  1
N2        0.05513   0.36551   0.65466                                 #  2
H*3       0.01146   0.33979   0.75984                                  #  3
H*4      -0.05591   0.38704   0.43627                                  #  4
N5        0.34862   0.39865   0.72864                                 #  5
H*6       0.27102   0.42395   0.51869                                  #  6
H*7       0.50742   0.39579   0.88486                                  #  7
N8        0.39760   0.33349   1.13608                                 #  8
O9        0.58243   0.33683   1.28067                                 #  9
O10       0.30986   0.30606   1.21196                                  # 10
#XC1       0.25364   0.36923   0.80918                                   # 11
#XN2       0.06425   0.36170   0.68399                                   # 12
#XH*3     -0.03699   0.33784   0.72795                                    # 13
#XH*4     -0.07350   0.39013   0.40344                                    # 14
#XN5       0.36629   0.39581   0.76013                                   # 15
#XH*6      0.26047   0.42784   0.48763                                    # 16
#XH*7      0.53637   0.40258   0.87249                                    # 17
#XN8       0.39061   0.33523   1.12021                                   # 18
#XO9       0.58348   0.33134   1.31227                                   # 19
#XO10      0.33985   0.30384   1.25085                                    # 20
```

```
N1+       0.30398   0.08072   0.89073                                  # 21
O2+       0.38388   0.15825   0.88385                                  # 22
O3+       0.26234   0.00371   0.73571                                  # 23
O4+       0.26572   0.08020   1.05263                                  # 24
#END

data_NO2F_NO3_4
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.77744E+02 E(coul)=-1.63730E+02 E(vdW)=-1.40136E+01 Density= 1.88325
;
_cell_length_a    9.575
_cell_length_b    8.706
_cell_length_c    6.693
_cell_angle_alpha    90.00
_cell_angle_beta    105.97
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        -0.20269  -0.69298   0.22857                                 #  1
N2        -0.12165  -0.62119   0.13071                                 #  2
H*3        -0.06214  -0.68589   0.05680                                 #  3
H*4        -0.11582  -0.50480   0.12562                                 #  4
N5        -0.28773  -0.63788   0.33353                                 #  5
H*6        -0.30083  -0.52339   0.35155                                 #  6
H*7        -0.34280  -0.71409   0.39955                                 #  7
N8        -0.19715  -0.86909   0.21870                                 #  8
O9        -0.27240  -0.93625   0.30956                                 #  9
O10        -0.11815  -0.92075   0.12119                                 # 10
#XC1       -0.20269  -0.69289   0.22857                                 # 11
#XN2       -0.11871  -0.63734   0.12684                                 # 12
#XH*3      -0.04061  -0.67175   0.03073                                 # 13
#XH*4      -0.11437  -0.48738   0.12415                                 # 14
#XN5       -0.28963  -0.65452   0.33557                                 # 15
#XH*6      -0.30336  -0.50637   0.35495                                 # 16
#XH*7      -0.36508  -0.70436   0.42696                                 # 17
#XN8       -0.19742  -0.86053   0.21918                                 # 18
#XO9       -0.26361  -0.95443   0.29849                                 # 19
#XO10      -0.12574  -0.94058   0.13013                                 # 20
```

```
N1+      -0.00564   0.24090   0.71574                    # 21
O2+       0.04882   0.31736   0.87891                    # 22
O3+       0.04758   0.25092   0.56330                    # 23
O4+      -0.11332   0.15442   0.70501                    # 24
#END

data_NO2F_NO3_5
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.77696E+02 E(coul)=-1.62384E+02 E(vdW)=-1.53120E+01 Density= 1.93460
;
_cell_length_a    6.217
_cell_length_b    6.380
_cell_length_c   13.166
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 212121'
_symmetry_Int_Tables_number  19
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2+x,1/2-y,-z
  3 -x,1/2+y,1/2-z
  4 1/2-x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.44715  -0.07183  -0.11891                    #  1
N2        0.62444   0.02084  -0.14700                    #  2
H*3       0.63145   0.18027  -0.14148                    #  3
H*4       0.75389  -0.05907  -0.17380                    #  4
N5        0.39795  -0.27058  -0.11848                    #  5
H*6       0.50159  -0.38370  -0.14202                    #  6
H*7       0.24869  -0.31220  -0.09327                    #  7
N8        0.26935   0.07542  -0.08050                    #  8
O9        0.10419  -0.01023  -0.05430                    #  9
O10       0.31454   0.26042  -0.08079                    # 10
#XC1       0.44724  -0.07190  -0.11893                    # 11
#XN2       0.61119   0.03879  -0.14385                    # 12
#XH*3      0.67336   0.20873  -0.14785                    # 13
#XH*4      0.77399  -0.06997  -0.17790                    # 14
#XN5       0.37810  -0.26112  -0.11449                    # 15
#XH*6      0.51625  -0.40159  -0.14544                    # 16
#XH*7      0.23087  -0.36061  -0.09211                    # 17
#XN8       0.27799   0.06826  -0.08237                    # 18
#XO9       0.09618   0.02002  -0.05156                    # 19
#XO10      0.28420   0.26194  -0.07524                    # 20
```

```
N1+       0.08566  -0.02930   0.66959                                  # 21
O2+       0.28668  -0.05713   0.67191                                  # 22
O3+      -0.00040   0.05721   0.59350                                  # 23
O4+      -0.02931  -0.08798   0.74336                                  # 24
#END
```

S10. Optimized crystal structure coordinates for formamidine – nitric acid (cocrystal form).

```
data_F_HNO3_1
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.16755E+01 E(coul)=-2.69802E+01 E(vdW)=-1.46953E+01 Density= 1.70136
;
_cell_length_a    3.998
_cell_length_b    8.675
_cell_length_c   12.054
_cell_angle_alpha    90.00
_cell_angle_beta     90.57
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.90586   0.10749   0.60248                                 #  1
N2        1.09841   0.23839   0.60577                                 #  2
H*3       1.01047   0.33574   0.57029                                 #  3
H*4       1.25867   0.25020   0.67076                                 #  4
N'5       0.96026  -0.00684   0.66743                                 #  5
H*6       0.79948  -0.09477   0.64958                                 #  6
H7        0.71064   0.11087   0.53736                                 #  7
#XC1       1.05062   0.15228   0.63301                                #  8
#XN2       1.11226   0.25472   0.61520                                #  9
#XH*3      1.04690   0.30535   0.58550                                # 10
#XH*4      1.20765   0.26353   0.64586                                # 11
#XN'5      1.01166   0.02314   0.67303                                # 12
#XH*6      0.79350  -0.10985   0.65351                                # 13
#XH7       0.66099   0.09522   0.51906                                # 14
N1+       0.44487  -0.10277   0.13418                                 # 15
O2+       0.23327  -0.08942   0.06355                                 # 16
O3+       0.55157  -0.21719   0.18060                                 # 17
O4+       0.59004   0.03830   0.16758                                 # 18
```

```
H*5+      0.75297   0.00756   0.22402                    # 19
#XN1+      0.38601  -0.14241   0.11888                    # 20
#XO2+      0.30406  -0.02199   0.07997                    # 21
#XO3+      0.60669  -0.13477   0.19038                    # 22
#XO4+      0.58376  -0.01984   0.17135                    # 23
#XH*5+     0.73801   0.01091   0.21879                    # 24
#XLP1+     0.46476  -0.12403   0.12094                    # 25
#XLP1-     0.39943  -0.11974   0.14289                    # 26
#XLP2+     0.31118  -0.13223   0.07504                    # 27
#XLP2-     0.25653  -0.12864   0.09341                    # 28
#XLP3+     0.42340  -0.21280   0.17914                    # 29
#XLP3-     0.54565  -0.22083   0.13806                    # 30
#XLP4+     0.71592   0.04847   0.14579                    # 31
#XLP4-     0.53088   0.06062   0.20797                    # 32
#END

data_F_HNO3_2
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.15973E+01 E(coul)=-2.75703E+01 E(vdW)=-1.40270E+01 Density= 1.72791
;
_cell_length_a    9.140
_cell_length_b    7.143
_cell_length_c    6.553
_cell_angle_alpha    90.00
_cell_angle_beta     74.19
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.40847   0.32121  -0.23659                    #  1
N2        0.30006   0.19146  -0.14358                    #  2
H*3       0.19043   0.23174  -0.09191                    #  3
H*4       0.32065   0.05660  -0.19002                    #  4
N'5       0.54053   0.27354  -0.35079                    #  5
H*6       0.60625   0.38911  -0.39896                    #  6
H7        0.37080   0.46660  -0.19784                    #  7
#XC1       0.38624   0.21473  -0.22500                    #  8
#XN2       0.28848   0.17129  -0.14976                    #  9
#XH*3      0.22657   0.21136  -0.11159                    # 10
```

```
#XH*4      0.29662   0.09795  -0.16417                    # 11
#XN'5      0.51772   0.23609  -0.33474                    # 12
#XH*6      0.62128   0.39292  -0.41107                    # 13
#XH7       0.37634   0.51054  -0.18944                    # 14
N1+       0.08664  -0.29901   0.73648                    # 15
O2+       0.14909  -0.15021   0.72661                    # 16
O3+      -0.03757  -0.34901   0.84372                    # 17
O4+       0.17314  -0.43601   0.60059                    # 18
H*5+      0.10743  -0.54583   0.62761                    # 19
#XN1+      0.06669  -0.24755   0.77490                    # 20
#XO2+      0.19011  -0.21670   0.66164                    # 21
#XO3+      0.02011  -0.40774   0.76472                    # 22
#XO4+      0.12458  -0.41799   0.65589                    # 23
#XH*5+     0.11391  -0.53587   0.62464                    # 24
#XLP1+     0.06460  -0.27793   0.73320                    # 25
#XLP1-     0.08192  -0.29286   0.77640                    # 26
#XLP2+     0.09436  -0.17075   0.74682                    # 27
#XLP2-     0.10885  -0.18324   0.78296                    # 28
#XLP3+    -0.00489  -0.31494   0.88467                    # 29
#XLP3-    -0.03731  -0.28701   0.80383                    # 30
#XLP4+     0.15455  -0.44260   0.52353                    # 31
#XLP4-     0.20362  -0.48488   0.64590                    # 32
#END

data_F_HNO3_3
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.12417E+01 E(coul)=-2.66546E+01 E(vdW)=-1.45870E+01 Density= 1.74294
;
_cell_length_a   11.600
_cell_length_b    4.535
_cell_length_c   15.516
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  8
_symmetry_space_group_name_H-M 'P BCA   '
_symmetry_Int_Tables_number  61
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,z
  3 x,1/2-y,1/2+z
  4 1/2-x,-y,1/2+z
  5 -x,-y,-z
  6 1/2+x,1/2-y,-z
  7 -x,1/2+y,1/2-z
  8 1/2+x,y,1/2-z
loop_
_atom_site_label
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
C1       -0.37350  -0.35730   0.67203                    #  1
N2       -0.41566  -0.10173   0.63669                    #  2
H*3       -0.42208  -0.08486   0.57207                    #  3
H*4       -0.47221   0.01597   0.67256                    #  4
N'5      -0.38900  -0.42317   0.75147                    #  5
H*6       -0.34780  -0.61525   0.76609                    #  6
H7       -0.32371  -0.49097   0.62587                    #  7
#XC1      -0.41133  -0.21571   0.67915                     #  8
#XN2      -0.42949  -0.08069   0.63458                     #  9
#XH*3     -0.42345  -0.08419   0.59472                     # 10
#XH*4     -0.45653  -0.00681   0.65216                     # 11
#XN'5     -0.40275  -0.36027   0.74594                     # 12
#XH*6     -0.34618  -0.63305   0.77347                     # 13
#XH7      -0.30354  -0.53740   0.62064                     # 14
N1+       0.62970   0.02786  -0.06402                    # 15
O2+       0.65779   0.23527  -0.02084                    # 16
O3+       0.57870  -0.19619  -0.04435                    # 17
O4+       0.66183   0.05223  -0.15147                    # 18
H*5+      0.63320  -0.13017  -0.17685                     # 19
#XN1+      0.62269   0.03747  -0.03533                     # 20
#XO2+      0.67299   0.24565  -0.06296                     # 21
#XO3+      0.60077  -0.15492  -0.08866                     # 22
#XO4+      0.64263  -0.00656  -0.12766                     # 23
#XH*5+     0.63601  -0.11284  -0.17472                      # 24
#XLP1+     0.61048   0.03678  -0.05621                     # 25
#XLP1-     0.63869  -0.00019  -0.05129                     # 26
#XLP2+     0.62634   0.15919  -0.01866                     # 27
#XLP2-     0.64994   0.12827  -0.01455                    # 28
#XLP3+     0.61268  -0.16934  -0.02459                     # 29
#XLP3-     0.55989  -0.10015  -0.03378                    # 30
#XLP4+     0.62372   0.09224  -0.17230                     # 31
#XLP4-     0.70363  -0.01247  -0.15839                    # 32
#END

data_F_HNO3_4
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.12337E+01 E(coul)=-2.68194E+01 E(vdW)=-1.44143E+01 Density= 1.69555
;
_cell_length_a    6.766
_cell_length_b    9.326
_cell_length_c    7.783
_cell_angle_alpha    90.00
_cell_angle_beta    121.33
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'C C     '
_symmetry_Int_Tables_number   9
loop_
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_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 x,-y,1/2+z
  3 1/2+x,1/2+y,z
  4 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        -0.19509   0.17792   0.38117                    #  1
N2        -0.17816   0.32436   0.40082                    #  2
H*3       -0.21693   0.38496   0.27995                    #  3
H*4       -0.20345   0.36859   0.50667                    #  4
N'5       -0.20485   0.09741   0.50990                    #  5
H*6       -0.20833  -0.00783   0.47310                    #  6
H7        -0.19318   0.13895   0.24839                    #  7
#XC1      -0.19515   0.24497   0.44224                    #  8
#XN2      -0.19348   0.34080   0.40257                    #  9
#XH*3     -0.20661   0.36800   0.32425                    # 10
#XH*4     -0.19805   0.36836   0.46054                    # 11
#XN'5     -0.20454   0.13258   0.52047                    # 12
#XH*6     -0.20901  -0.02127   0.48115                    # 13
#XH7      -0.18190   0.11549   0.22377                    # 14
N1+       0.29821   0.17522   0.37167                    # 15
O2+       0.32186   0.13998   0.52959                    # 16
O3+       0.24388   0.10504   0.22198                    # 17
O4+       0.34113   0.32210   0.36108                    # 18
H*5+      0.31486   0.33252   0.22617                    # 19
#XN1+     0.28772   0.13002   0.38740                    # 20
#XO2+     0.34226   0.21050   0.52354                    # 21
#XO3+     0.27154   0.18438   0.23673                    # 22
#XO4+     0.31878   0.27324   0.32767                    # 23
#XH*5+    0.31748   0.33199   0.23890                    # 24
#XLP1+    0.26050   0.16094   0.35829                    # 25
#XLP1-    0.32309   0.15272   0.37821                    # 26
#XLP2+    0.27513   0.12096   0.45890                    # 27
#XLP2-    0.32750   0.11408   0.47557                    # 28
#XLP3+    0.30843   0.08304   0.28815                    # 29
#XLP3-    0.19129   0.09842   0.25086                    # 30
#XLP4+    0.25598   0.35428   0.31990                    # 31
#XLP4-    0.43328   0.33101   0.37634                    # 32
#END

data_F_HNO3_5
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.12110E+01 E(coul)=-2.75283E+01 E(vdW)=-1.36827E+01 Density= 1.66741
;
_cell_length_a    7.687
_cell_length_b    7.671
```

```
_cell_length_c    9.417
_cell_angle_alpha    90.00
_cell_angle_beta     50.20
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.22057  -0.22823   0.69199                    #  1
N2         0.20480  -0.21633   0.84529                    #  2
H*3        0.22936  -0.32407   0.89182                    #  3
H*4        0.24383  -0.10010   0.86955                    #  4
N'5        0.24710  -0.09366   0.59933                    #  5
H*6        0.24665  -0.12846   0.49513                    #  6
H7         0.20226  -0.36270   0.66205                    #  7
#XC1       0.22789  -0.16717   0.75498                    #  8
#XN2       0.22072  -0.20881   0.85334                    #  9
#XH*3      0.22434  -0.28314   0.87791                    # 10
#XH*4      0.23250  -0.14877   0.87489                    # 11
#XN'5      0.24792  -0.08344   0.63380                    # 12
#XH*6      0.24843  -0.11994   0.48095                    # 13
#XH7       0.18768  -0.39169   0.64622                    # 14
N1+        0.21576   0.76387   0.18978                    # 15
O2+        0.24020   0.91251   0.14037                    # 16
O3+        0.18104   0.63340   0.13813                    # 17
O4+        0.23023   0.73935   0.33047                    # 18
H*5+       0.20716   0.61435   0.35397                    # 19
#XN1+      0.21354   0.78287   0.14522                    # 20
#XO2+      0.24698   0.89985   0.20802                    # 21
#XO3+      0.19254   0.63897   0.21207                    # 22
#XO4+      0.21878   0.71358   0.28739                    # 23
#XH*5+     0.20939   0.62610   0.35218                    # 24
#XLP1+     0.24443   0.75893   0.15466                    # 25
#XLP1-     0.18176   0.76623   0.19061                    # 26
#XLP2+     0.25270   0.85442   0.11026                    # 27
#XLP2-     0.20028   0.86053   0.14033                    # 28
#XLP3+     0.12935   0.68534   0.15338                    # 29
#XLP3-     0.24662   0.67168   0.08610                    # 30
#XLP4+     0.31895   0.71504   0.30039                    # 31
#XLP4-     0.14144   0.73572   0.40223                    # 32
#END
```

S11. Optimized crystal structure coordinates for azidoformamidine – nitric acid (cocrystal form).

```
data_N3F_HNO3_1
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-3.82087E+01 E(coul)=-2.39342E+01 E(vdW)=-1.42745E+01 Density= 1.66378
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_cell_length_a    4.828
_cell_length_b    9.041
_cell_length_c   14.227
_cell_angle_alpha    90.00
_cell_angle_beta    107.81
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.24458   0.43811  -0.10780                                  #  1
N'2       0.41143   0.42310  -0.16187                                  #  2
H*3        0.49497   0.31881  -0.15751                                   #  3
N4        0.16294   0.33462  -0.05017                                  #  4
N'5       0.10303   0.57507  -0.10284                                  #  5
N6        0.15387   0.67491  -0.15568                                  #  6
N'7       0.18308   0.77419  -0.20021                                  #  7
H*8        0.28505   0.24219  -0.03266                                   #  8
H*9        0.07197   0.37154   0.00067                                   #  9
#XC1       0.20896   0.43215  -0.09228                                    # 10
#XN'2      0.40300   0.44569  -0.17149                                    # 11
#XH*3       0.50319   0.32510  -0.16174                                     # 12
#XN4       0.20082   0.35360  -0.04620                                    # 13
#XN'5      0.08972   0.56868  -0.09250                                    # 14
#XN6       0.16036   0.66329  -0.15496                                    # 15
#XN'7      0.16318   0.78416  -0.19258                                    # 16
#XH*8       0.28365   0.24466  -0.03054                                     # 17
#XH*9       0.06364   0.37180   0.00505                                     # 18
#XLP1+      0.25844   0.46923  -0.10264                                      # 19
#XLP1-      0.20355   0.43879  -0.11296                                     # 20
#XLP2+      0.40179   0.40723  -0.14513                                      # 21
#XLP2-      0.41509   0.43665  -0.16244                                     # 22
#XLP4+      0.27356   0.34348  -0.01076                                      # 23
#XLP4-      0.06084   0.30378  -0.07473                                     # 24
```

```
#XLP5+     0.15413   0.58542  -0.06812                    # 25
#XLP5-     0.00869   0.55703  -0.11279                    # 26
#XLP6+     0.13877   0.67270  -0.15352                    # 27
#XLP6-     0.14835   0.67662  -0.14780                    # 28
#XLP7+     0.24363   0.80857  -0.18384                    # 29
#XLP7-     0.10914   0.78491  -0.22778                    # 30
N1+       0.35607   0.54349   0.59740                    # 31
O2+       0.37441   0.62581   0.53341                    # 32
O3+       0.23036   0.42597   0.59217                    # 33
O4+       0.50599   0.59309   0.69359                    # 34
H*5+      0.46974   0.51527   0.73574                    # 35
#XN1+      0.31429   0.53579   0.56451                    # 36
#XO2+      0.44604   0.64903   0.57984                    # 37
#XO3+      0.31849   0.46517   0.63874                    # 38
#XO4+      0.44321   0.55420   0.67132                    # 39
#XH*5+     0.47363   0.52278   0.73205                    # 40
#XLP1+     0.36923   0.52445   0.58604                    # 41
#XLP1-     0.30205   0.54436   0.58716                    # 42
#XLP2+     0.35722   0.57110   0.53507                    # 43
#XLP2-     0.30102   0.58776   0.53601                    # 44
#XLP3+     0.16914   0.46795   0.57160                    # 45
#XLP3-     0.29486   0.43070   0.56951                    # 46
#XLP4+     0.61809   0.56487   0.70848                    # 47
#XLP4-     0.42780   0.62126   0.71166                    # 48
#END

data_N3F_HNO3_2
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-3.81507E+01 E(coul)=-2.39011E+01 E(vdW)=-1.42496E+01 Density= 1.68659
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_cell_length_a    8.357
_cell_length_b    7.673
_cell_length_c    9.198
_cell_angle_alpha    90.00
_cell_angle_beta     81.45
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

```
C1        0.68570   0.07536   0.80241                 #  1
N'2       0.80508   0.12779   0.70915                 #  2
H*3       0.85302   0.02945   0.64177                 #  3
N4        0.61572  -0.08755   0.81840                 #  4
N'5       0.59983   0.19146   0.90739                 #  5
N6        0.64995   0.34461   0.89830                 #  6
N'7       0.68410   0.48720   0.90135                 #  7
H*8       0.68067  -0.18848   0.77038                 #  8
H*9       0.54166  -0.11364   0.91311                 #  9
#XC1      0.65869   0.05126   0.82158                 # 10
#XN'2     0.80385   0.15917   0.71207                 # 11
#XH*3     0.85947   0.04027   0.63956                 # 12
#XN4      0.63599  -0.07326   0.83092                 # 13
#XN'5     0.58793   0.17350   0.91759                 # 14
#XN6      0.65355   0.33329   0.89138                 # 15
#XN'7     0.66929   0.48715   0.91895                 # 16
#XH*8     0.67898  -0.18862   0.77464                 # 17
#XH*9     0.53502  -0.11861   0.91954                 # 18
#XLP1+    0.69137   0.09872   0.82636                 # 19
#XLP1-    0.66389   0.08045   0.80081                 # 20
#XLP2+    0.79280   0.09402   0.72102                 # 21
#XLP2-    0.80730   0.14105   0.71638                 # 22
#XLP4+    0.66405  -0.12007   0.86062                 # 23
#XLP4-    0.56654  -0.09171   0.78006                 # 24
#XLP5+    0.61536   0.16363   0.95104                 # 25
#XLP5-    0.54909   0.18292   0.89405                 # 26
#XLP6+    0.64029   0.33964   0.90120                 # 27
#XLP6-    0.64351   0.33714   0.90962                 # 28
#XLP7+    0.71236   0.50247   0.93617                 # 29
#XLP7-    0.65212   0.52565   0.88183                 # 30
N1+      -0.09883   0.79415   0.03141                 # 31
O2+      -0.21649   0.86667   0.09404                 # 32
O3+      -0.02497   0.66911   0.06786                 # 33
O4+      -0.03840   0.86782  -0.10645                 # 34
H*5+      0.05496   0.79516  -0.14175                 # 35
#XN1+    -0.12571   0.77871   0.07622                 # 36
#XO2+    -0.18683   0.90148   0.02767                 # 37
#XO3+    -0.00592   0.72079  -0.00271                 # 38
#XO4+    -0.03399   0.82187  -0.06761                 # 39
#XH*5+    0.04631   0.80227  -0.13883                 # 40
#XLP1+   -0.11655   0.76724   0.03867                 # 41
#XLP1-   -0.08995   0.79710   0.05688                 # 42
#XLP2+   -0.19438   0.80578   0.09534                 # 43
#XLP2-   -0.17213   0.83075   0.11058                 # 44
#XLP3+   -0.03685   0.71686   0.10718                 # 45
#XLP3-   -0.08661   0.66099   0.07310                 # 46
#XLP4+   -0.05999   0.82918  -0.15371                 # 47
#XLP4-    0.01534   0.91374  -0.10212                 # 48
#END

data_N3F_HNO3_3
_chemical_name_systematic
```

```
;RAS NH3 PVDZ

E(total)=-3.80605E+01 E(coul)=-2.30710E+01 E(vdW)=-1.49895E+01 Density= 1.68734
;
_cell_length_a    4.897
_cell_length_b   10.651
_cell_length_c    5.635
_cell_angle_alpha    94.16
_cell_angle_beta     92.98
_cell_angle_gamma    95.08
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.87855  -0.19270   0.30493                          #  1
N'2       0.86553  -0.30568   0.20790                          #  2
H*3        0.72013  -0.36392   0.27905                          #  3
N4        0.72255  -0.14289   0.47892                          #  4
N'5       1.06751  -0.09512   0.23231                          #  5
N6        1.21173  -0.12953   0.06820                          #  6
N'7       1.35436  -0.14898  -0.07917                          #  7
H*8        0.61707  -0.20452   0.57594                          #  8
H*9        0.79188  -0.05829   0.56367                          #  9
#XC1       0.86887  -0.16802   0.33916                          # 10
#XN'2      0.89394  -0.30345   0.17424                          # 11
#XH*3       0.73007  -0.36884   0.26715                          # 12
#XN4       0.76780  -0.15091   0.48083                          # 13
#XN'5      1.06009  -0.08363   0.25727                          # 14
#XN6       1.19485  -0.13467   0.07642                          # 15
#XN'7      1.37027  -0.13255  -0.06928                          # 16
#XH*8       0.62221  -0.20176   0.57916                          # 17
#XH*9       0.79287  -0.05154   0.57247                          # 18
#XLP1+      0.93771  -0.18675   0.30110                          # 19
#XLP1-     0.86414  -0.17923   0.28983                          # 20
#XLP2+      0.84786  -0.29345   0.25218                          # 21
#XLP2-     0.88867  -0.30416   0.19986                          # 22
#XLP4+      0.79655  -0.15780   0.57002                          # 23
#XLP4-     0.62476  -0.12625   0.43264                          # 24
#XLP5+      1.12336  -0.08830   0.30741                          # 25
#XLP5-     1.00319  -0.06773   0.21207                          # 26
#XLP6+      1.20512  -0.12222   0.07285                          # 27
#XLP6-     1.21833  -0.12101   0.08416                          # 28
#XLP7+      1.44025  -0.15341  -0.05619                          # 29
#XLP7-     1.33163  -0.13566  -0.15147                          # 30
```

```
N1+       1.22920   0.44654   0.27051                                  # 31
O2+       1.41360   0.38820   0.33700                                  # 32
O3+       0.98233   0.42028   0.26438                                  # 33
O4+       1.31739   0.56422   0.18668                                  # 34
H*5+      1.14616   0.59856   0.14069                                   # 35
#XN1+      1.21855   0.40790   0.30003                                    # 36
#XO2+      1.45467   0.44489   0.29647                                    # 37
#XO3+      1.05705   0.47988   0.22521                                    # 38
#XO4+      1.23920   0.53223   0.20355                                    # 39
#XH*5+     1.16263   0.59568   0.14478                                     # 40
#XLP1+     1.21090   0.44050   0.31048                                     # 41
#XLP1-     1.21285   0.42493   0.24871                                    # 42
#XLP2+     1.31466   0.38911   0.35656                                     # 43
#XLP2-     1.31629   0.37608   0.30489                                    # 44
#XLP3+     1.03707   0.38524   0.22863                                     # 45
#XLP3-     1.03342   0.41438   0.34422                                    # 46
#XLP4+     1.31178   0.60496   0.25901                                     # 47
#XLP4-     1.31730   0.56085   0.08405                                    # 48
#END

data_N3F_HNO3_4
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-3.78296E+01 E(coul)=-2.42777E+01 E(vdW)=-1.35519E+01 Density= 1.64292
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_cell_length_a   15.319
_cell_length_b   11.173
_cell_length_c    3.627
_cell_angle_alpha    90.00
_cell_angle_beta     74.70
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.65110   1.00722   0.71382                                  #  1
N'2       0.73294   0.99578   0.51235                                  #  2
H*3        0.75676   1.07268   0.36937                                   #  3
N4        0.59576   1.10651   0.76554                                  #  4
N'5       0.60421   0.91075   0.93895                                  #  5
N6        0.64984   0.81766   0.92371                                  #  6
```

```
N'7       0.68399   0.72829   0.93335                    #  7
H*8       0.61371   1.17350   0.57390                    #  8
H*9       0.52867   1.09405   0.87911                    #  9
#XC1      0.63112   1.01767   0.75255                    # 10
#XN'2     0.73739   0.97672   0.53355                    # 11
#XH*3     0.76139   1.06625   0.36231                    # 12
#XN4      0.59719   1.08928   0.72281                    # 13
#XN'5     0.59313   0.91882   0.95071                    # 14
#XN6      0.65175   0.82650   0.91129                    # 15
#XN'7     0.67223   0.72341   0.95984                    # 16
#XH*8     0.61126   1.17206   0.57591                    # 17
#XH*9     0.52313   1.09533   0.88852                    # 18
#XLP1+    0.64553   0.98247   0.70540                    # 19
#XLP1-    0.64790   1.00890   0.76761                    # 20
#XLP2+    0.71790   1.01229   0.51438                    # 21
#XLP2-    0.73259   0.98466   0.51252                    # 22
#XLP4+    0.58027   1.09836   0.61688                    # 23
#XLP4-    0.60204   1.13422   0.89160                    # 24
#XLP5+    0.58149   0.90518   0.86771                    # 25
#XLP5-    0.59736   0.93051   1.05537                    # 26
#XLP6+    0.64529   0.82101   0.94150                    # 27
#XLP6-    0.64152   0.81825   0.92905                    # 28
#XLP7+    0.67680   0.69946   0.86358                    # 29
#XLP7-    0.69354   0.72033   1.03876                    # 30
N1+       0.06693  -0.88297   0.29080                    # 31
O2+       0.00757  -0.81220   0.29837                    # 32
O3+       0.07871  -0.98311   0.15642                    # 33
O4+       0.13298  -0.84160   0.46775                    # 34
H*5+      0.17524  -0.90834   0.43711                    # 35
#XN1+     0.04311  -0.88923   0.24035                    # 36
#XO2+     0.03955  -0.79284   0.38301                    # 37
#XO3+     0.10865  -0.95013   0.25860                    # 38
#XO4+     0.12135  -0.87454   0.39700                    # 39
#XH*5+    0.17145  -0.90190   0.44056                    # 40
#XLP1+    0.06669  -0.88422   0.22032                    # 41
#XLP1-    0.05329  -0.89702   0.31391                    # 42
#XLP2+    0.02099  -0.84641   0.21156                    # 43
#XLP2-    0.00978  -0.85711   0.28985                    # 44
#XLP3+    0.04672  -0.97497   0.24172                    # 45
#XLP3-    0.07179  -0.95103   0.06658                    # 46
#XLP4+    0.16441  -0.82366   0.35626                    # 47
#XLP4-    0.12646  -0.85989   0.62134                    # 48
#END

data_N3F_HNO3_5
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-3.78042E+01 E(coul)=-2.25145E+01 E(vdW)=-1.52898E+01 Density= 1.72432
;
_cell_length_a    9.204
_cell_length_b    6.892
```

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_cell_length_c    9.620
_cell_angle_alpha    90.00
_cell_angle_beta     69.23
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.58172   0.58789   0.68649                    #  1
N'2       0.58903   0.63780   0.81201                    #  2
H*3       0.63517   0.53055   0.85663                    #  3
N4        0.63034   0.41843   0.60745                    #  4
N'5       0.52139   0.71605   0.60378                    #  5
N6        0.47958   0.87720   0.66332                    #  6
N'7       0.43757   1.02780   0.70580                    #  7
H*8       0.64893   0.30293   0.66343                    #  8
H*9       0.59117   0.38967   0.52385                    #  9
#XC1      0.58344   0.56339   0.65731                    # 10
#XN'2     0.58294   0.67211   0.81330                    # 11
#XH*3     0.63192   0.54166   0.86365                    # 12
#XN4      0.60488   0.42908   0.62440                    # 13
#XN'5     0.52152   0.69696   0.58995                    # 14
#XN6      0.48527   0.86506   0.66663                    # 15
#XN'7     0.43029   1.02791   0.68979                    # 16
#XH*8     0.64605   0.30250   0.66120                    # 17
#XH*9     0.58990   0.38448   0.51647                    # 18
#XLP1+    0.55329   0.60945   0.68949                    # 19
#XLP1-    0.59553   0.59735   0.66810                    # 20
#XLP2+    0.58994   0.60117   0.79612                    # 21
#XLP2-    0.57933   0.65104   0.81393                    # 22
#XLP4+    0.56710   0.36901   0.63964                    # 23
#XLP4-    0.69539   0.42715   0.57050                    # 24
#XLP5+    0.47578   0.67710   0.60738                    # 25
#XLP5-    0.56503   0.71693   0.56078                    # 26
#XLP6+    0.48335   0.87297   0.65390                    # 27
#XLP6-    0.47404   0.86857   0.65504                    # 28
#XLP7+    0.38676   1.03526   0.72602                    # 29
#XLP7-    0.46947   1.07800   0.68461                    # 30
N1+      -0.20888   0.60837   0.12394                    # 31
O2+      -0.26211   0.57589   0.25492                    # 32
O3+      -0.24410   0.54372   0.02273                    # 33
O4+      -0.08579   0.74371   0.08316                    # 34
```

```
H*5+     -0.05659   0.75333  -0.02438                    # 35
#XN1+     -0.24867   0.56672   0.14622                    # 36
#XO2+     -0.20287   0.64086   0.23459                    # 37
#XO3+     -0.18073   0.61682   0.01667                    # 38
#XO4+     -0.12110   0.69869   0.06792                    # 39
#XH*5+    -0.05897   0.75284  -0.01433                    # 40
#XLP1+    -0.23787   0.61173   0.12781                    # 41
#XLP1-    -0.20928   0.57112   0.12289                    # 42
#XLP2+    -0.28314   0.57218   0.21331                    # 43
#XLP2-    -0.25922   0.53821   0.20920                    # 44
#XLP3+    -0.23643   0.49253   0.05837                    # 45
#XLP3-    -0.28993   0.56853   0.06757                    # 46
#XLP4+    -0.10731   0.82016   0.07546                    # 47
#XLP4-    -0.02633   0.70512   0.06154                    # 48
#END
```

S12. Optimized crystal structure coordinates for guanidine – nitric acid (cocrystal form).

```
data_G_HNO3_1
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.82115E+01 E(coul)=-3.23389E+01 E(vdW)=-1.58725E+01 Density= 1.73117
;
_cell_length_a    7.294
_cell_length_b   14.783
_cell_length_c    4.350
_cell_angle_alpha    90.00
_cell_angle_beta     87.29
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.71173  -0.34287  -0.22440                   #  1
N'2       0.61954  -0.30664   0.00249                   #  2
H*3       0.69910  -0.26387   0.12323                    #  3
N4        0.63398  -0.41098  -0.39765                   #  4
H*5       0.66320  -0.40730  -0.62744                    #  5
H*6       0.49825  -0.41885  -0.34373                    #  6
N7        0.89061  -0.32159  -0.33045                   #  7
H*8       0.95972  -0.28146  -0.18732                    #  8
```

```
H*9       0.96640  -0.37470  -0.41143                    #  9
#XC1       0.71294  -0.35395  -0.27884                    # 10
#XN'2      0.60105  -0.31067  -0.00234                    # 11
#XH*3      0.67865  -0.26422   0.13632                    # 12
#XN4       0.63555  -0.40487  -0.42044                    # 13
#XH*5      0.65466  -0.40766  -0.63126                    # 14
#XH*6      0.50955  -0.41659  -0.34829                    # 15
#XN7       0.88386  -0.32874  -0.32028                    # 16
#XH*8      0.95962  -0.28149  -0.18974                    # 17
#XH*9      0.96756  -0.37050  -0.40787                    # 18
#XLP1+     0.70421  -0.33153  -0.25274                    # 19
#XLP1-     0.70943  -0.35823  -0.19980                    # 20
#XLP2+     0.59422  -0.30463  -0.01967                    # 21
#XLP2-     0.62753  -0.31632   0.02172                    # 22
#XLP4+     0.59299  -0.38423  -0.49458                    # 23
#XLP4-     0.66277  -0.44359  -0.36582                    # 24
#XLP7+     0.88898  -0.30593  -0.42660                    # 25
#XLP7-     0.91983  -0.34550  -0.24130                    # 26
N1+       0.20455   0.57560   0.12597                    # 27
O2+       0.05942   0.55389   0.24501                    # 28
O3+       0.28656   0.54628  -0.10230                    # 29
O4+       0.29179   0.64668   0.27903                    # 30
H*5+      0.40521   0.65574   0.15541                    # 31
#XN1+      0.16773   0.55335   0.09136                    # 32
#XO2+      0.10207   0.58804   0.31752                    # 33
#XO3+      0.31732   0.58406   0.00091                    # 34
#XO4+      0.29228   0.62414   0.19110                    # 35
#XH*5+     0.39475   0.65511   0.16758                    # 36
#XLP1+     0.18553   0.57531   0.07773                    # 37
#XLP1-     0.20931   0.55838   0.12637                    # 38
#XLP2+     0.08727   0.55202   0.13712                    # 39
#XLP2-     0.10716   0.53785   0.17781                    # 40
#XLP3+     0.26315   0.52212  -0.02509                    # 41
#XLP3-     0.21865   0.55381  -0.11611                    # 42
#XLP4+     0.27949   0.68095   0.22005                    # 43
#XLP4-     0.34684   0.63297   0.35782                    # 44
#END

data_G_HNO3_2
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.80180E+01 E(coul)=-3.16561E+01 E(vdW)=-1.63619E+01 Density= 1.72579
;
_cell_length_a   14.972
_cell_length_b    4.155
_cell_length_c    7.564
_cell_angle_alpha    90.00
_cell_angle_beta     92.87
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
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_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       -0.15536  -0.07925   0.20889                    #  1
N'2      -0.18506  -0.15167   0.05163                    #  2
H*3       -0.23486  -0.31908   0.05381                    #  3
N4       -0.08052   0.11806   0.23448                    #  4
H*5       -0.08414   0.28067   0.33376                    #  5
H*6       -0.06168   0.21694   0.11970                    #  6
N7       -0.19042  -0.17500   0.36864                    #  7
H*8       -0.23698  -0.35105   0.35636                    #  8
H*9       -0.14446  -0.21515   0.46923                    #  9
#XC1      -0.14411  -0.04023   0.23220                    # 10
#XN'2     -0.17949  -0.12942   0.04117                    # 11
#XH*3      -0.23289  -0.30795   0.03453                    # 12
#XN4      -0.08635   0.13839   0.24148                    # 13
#XH*5      -0.08301   0.29300   0.32898                    # 14
#XH*6      -0.06481   0.20954   0.12875                    # 15
#XN7      -0.18299  -0.17960   0.36258                    # 16
#XH*8      -0.23692  -0.34893   0.35713                    # 17
#XH*9      -0.14869  -0.21738   0.46745                    # 18
#XLP1+     -0.16544  -0.04185   0.20945                    # 19
#XLP1-     -0.14050  -0.10473   0.20380                    # 20
#XLP2+     -0.18458  -0.10454   0.04018                    # 21
#XLP2-     -0.17655  -0.18115   0.05401                    # 22
#XLP4+     -0.10192   0.25682   0.22925                    # 23
#XLP4-     -0.05165   0.04435   0.25521                    # 24
#XLP7+     -0.20446  -0.08509   0.39544                    # 25
#XLP7-     -0.17067  -0.29305   0.36705                    # 26
N1+       0.58481  -0.21229   0.27107                    # 27
O2+       0.57468  -0.10024   0.41490                    # 28
O3+       0.55571  -0.12542   0.12605                    # 29
O4+       0.63947  -0.48915   0.27355                    # 30
H*5+       0.64077  -0.54819   0.14902                    # 31
#XN1+      0.56822  -0.12341   0.28190                    # 32
#XO2+      0.60090  -0.23344   0.41519                    # 33
#XO3+      0.58563  -0.26896   0.14642                    # 34
#XO4+      0.62058  -0.40790   0.23840                    # 35
#XH*5+      0.64082  -0.54346   0.16081                    # 36
#XLP1+     0.58800  -0.15299   0.26405                    # 37
#XLP1-     0.56774  -0.20502   0.26865                    # 38
#XLP2+     0.57356  -0.05491   0.35313                    # 39
#XLP2-     0.55661  -0.09844   0.35698                    # 40
```

```
#XLP3+     0.53232  -0.13348   0.17333                    # 41
#XLP3-     0.57024  -0.03610   0.16471                    # 42
#XLP4+     0.67559  -0.45756   0.25670                    # 43
#XLP4-     0.61821  -0.60494   0.26974                    # 44
#END

data_G_HNO3_3
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.78522E+01 E(coul)=-3.15133E+01 E(vdW)=-1.63389E+01 Density= 1.72012
;
_cell_length_a    7.572
_cell_length_b   14.845
_cell_length_c    4.195
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 212121'
_symmetry_Int_Tables_number  19
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2+x,1/2-y,-z
  3 -x,1/2+y,1/2-z
  4 1/2-x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.44877   0.40482   0.57766                   #  1
N'2       0.29548   0.43599   0.64875                   #  2
H*3       0.30385   0.48571   0.81604                    #  3
N4        0.46486   0.32970   0.38028                   #  4
H*5       0.56499   0.33279   0.22026                    #  5
H*6       0.34800   0.31202   0.28069                    #  6
N7        0.61273   0.43842   0.67506                   #  7
H*8       0.60619   0.48500   0.85068                    #  8
H*9       0.70689   0.39116   0.71446                    #  9
#XC1      0.47065   0.39337   0.53890                     # 10
#XN'2     0.28435   0.43053   0.62644                     # 11
#XH*3      0.28436   0.48393   0.80477                     # 12
#XN4      0.47269   0.33555   0.36039                     # 13
#XH*5      0.56010   0.33172   0.20797                     # 14
#XH*6      0.35743   0.31506   0.28819                     # 15
#XN7      0.60566   0.43099   0.67934                    # 16
#XH*8      0.60696   0.48493   0.84858                     # 17
#XH*9      0.70568   0.39543   0.71677                     # 18
#XLP1+     0.45080   0.41503   0.54091                      # 19
#XLP1-     0.44161   0.38986   0.60242                     # 20
```

```
#XLP2+     0.28413   0.43572   0.60194                    # 21
#XLP2-     0.29663   0.42734   0.67772                    # 22
#XLP4+     0.46293   0.35159   0.24340                    # 23
#XLP4-     0.48147   0.30030   0.45265                    # 24
#XLP7+     0.64165   0.45250   0.58666                    # 25
#XLP7-     0.60813   0.41830   0.79140                    # 26
N1+       -0.03480   0.33541   0.21041                   # 27
O2+       -0.17906   0.32540   0.09746                   # 28
O3+        0.10769   0.30685   0.12394                   # 29
O4+       -0.03316   0.38914   0.48799                   # 30
H*5+       0.09117   0.39047   0.54771                    # 31
#XN1+     -0.04685   0.31910   0.12126                    # 32
#XO2+     -0.17737   0.35118   0.23100                    # 33
#XO3+      0.08962   0.33626   0.26777                    # 34
#XO4+      0.00049   0.37058   0.40667                    # 35
#XH*5+     0.07941   0.39051   0.54292                    # 36
#XLP1+    -0.02733   0.33892   0.15194                    # 37
#XLP1-    -0.03390   0.31826   0.20218                    # 38
#XLP2+    -0.11733   0.32464   0.05308                    # 39
#XLP2-    -0.12282   0.30735   0.09510                    # 40
#XLP3+     0.05834   0.28314   0.13003                    # 41
#XLP3-     0.07062   0.32182   0.03601                    # 42
#XLP4+    -0.01301   0.42572   0.45908                    # 43
#XLP4-    -0.03159   0.36718   0.60139                    # 44
#END

data_G_HNO3_4
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.78398E+01 E(coul)=-3.07353E+01 E(vdW)=-1.71045E+01 Density= 1.77176
;
_cell_length_a    7.869
_cell_length_b    9.252
_cell_length_c    6.287
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 212121'
_symmetry_Int_Tables_number  19
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2+x,1/2-y,-z
  3 -x,1/2+y,1/2-z
  4 1/2-x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

```
C1        0.36516   0.19216  -0.27748                    #  1
N'2       0.24492   0.21021  -0.14186                    #  2
H*3       0.27906   0.28183  -0.02607                    #  3
N4        0.35139   0.08668  -0.43488                    #  4
H*5       0.39530   0.11640  -0.58000                    #  5
H*6       0.23360   0.04261  -0.44009                    #  6
N7        0.51751   0.26954  -0.29122                    #  7
H*8       0.54206   0.33323  -0.16411                    #  8
H*9       0.61981   0.21101  -0.33800                    #  9
#XC1      0.37726   0.17993  -0.31673                    # 10
#XN'2     0.23161   0.20070  -0.15155                    # 11
#XH*3     0.26040   0.27606  -0.02329                    # 12
#XN4      0.35141   0.09806  -0.44812                    # 13
#XH*5     0.38847   0.11440  -0.58514                    # 14
#XH*6     0.24251   0.04872  -0.43928                    # 15
#XN7      0.51473   0.25651  -0.28826                    # 16
#XH*8     0.54221   0.33335  -0.16578                    # 17
#XH*9     0.61816   0.21733  -0.33413                    # 18
#XLP1+    0.35492   0.21005  -0.29568                    # 19
#XLP1-    0.36949   0.16648  -0.26573                    # 20
#XLP2+    0.22392   0.20981  -0.16357                    # 21
#XLP2-    0.25547   0.19567  -0.12921                    # 22
#XLP4+    0.30984   0.12645  -0.50478                    # 23
#XLP4-    0.39152   0.04065  -0.41389                    # 24
#XLP7+    0.51607   0.30052  -0.35217                    # 25
#XLP7-    0.54801   0.23225  -0.22921                    # 26
N1+      -0.11280   0.04749   0.64879                    # 27
O2+      -0.25498   0.03144   0.58402                    # 28
O3+       0.01020  -0.03142   0.63679                    # 29
O4+      -0.08683   0.17986   0.75552                    # 30
H*5+      0.03240   0.17568   0.79691                    # 31
#XN1+    -0.13170   0.00801   0.61280                    # 32
#XO2+    -0.24167   0.09490   0.63551                    # 33
#XO3+     0.00631   0.04215   0.68928                    # 34
#XO4+    -0.06316   0.13209   0.72933                    # 35
#XH*5+    0.02120   0.17649   0.79332                    # 36
#XLP1+   -0.10575   0.03917   0.61079                    # 37
#XLP1-   -0.11805   0.02168   0.66245                    # 38
#XLP2+   -0.19783   0.01204   0.56222                    # 39
#XLP2-   -0.20812  -0.00259   0.60543                    # 40
#XLP3+   -0.04452  -0.05598   0.66300                    # 41
#XLP3-   -0.02152  -0.02325   0.56634                    # 42
#XLP4+   -0.05574   0.22198   0.70019                    # 43
#XLP4-   -0.09056   0.17245   0.84650                    # 44
#END

data_G_HNO3_5
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.75778E+01 E(coul)=-3.08894E+01 E(vdW)=-1.66884E+01 Density= 1.73761
;
```

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_cell_length_a    4.804
_cell_length_b   11.688
_cell_length_c    8.313
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 212121'
_symmetry_Int_Tables_number  19
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2+x,1/2-y,-z
  3 -x,1/2+y,1/2-z
  4 1/2-x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.85910   0.06932   0.51989                    #  1
N'2       0.94735   0.07919   0.66510                    #  2
H*3       1.10566   0.02332   0.68804                    #  3
N4        0.62320   0.12891   0.46965                    #  4
H*5       0.63498   0.16219   0.35726                    #  5
H*6       0.55860   0.18640   0.55288                    #  6
N7        0.97576   0.00346   0.39659                    #  7
H*8       1.12363  -0.05226   0.43356                    #  8
H*9       0.83694  -0.03224   0.31966                    #  9
#XC1      0.82415   0.07724   0.49409                    # 10
#XN'2     0.92922   0.08882   0.67072                    # 11
#XH*3     1.09862   0.03116   0.70286                    # 12
#XN4      0.64123   0.13430   0.45993                    # 13
#XH*5     0.63105   0.16733   0.35938                    # 14
#XH*6     0.56880   0.18203   0.54615                    # 15
#XN7      0.95249   0.00311   0.40300                    # 16
#XH*8     1.12342  -0.05171   0.43255                    # 17
#XH*9     0.85008  -0.03254   0.32130                    # 18
#XLP1+    0.88980   0.08188   0.51260                    # 19
#XLP1-    0.81310   0.06165   0.52937                    # 20
#XLP2+    0.94458   0.09744   0.66714                    # 21
#XLP2-    0.92148   0.06868   0.66846                    # 22
#XLP4+    0.68710   0.17686   0.44985                    # 23
#XLP4-    0.53539   0.09933   0.46581                    # 24
#XLP7+    1.01876   0.02806   0.35784                    # 25
#XLP7-    0.91637  -0.03606   0.41871                    # 26
N1+       0.62487   0.30623  -0.15264                    # 27
O2+       0.58388   0.39153  -0.07589                    # 28
O3+       0.46367   0.24563  -0.22621                    # 29
O4+       0.90672   0.27226  -0.15666                    # 30
H*5+      0.90373   0.20324  -0.22239                    # 31
#XN1+     0.54026   0.32287  -0.14533                    # 32
```

```
#XO2+      0.71902   0.37474  -0.07828                    # 33
#XO3+      0.61942   0.23744  -0.21839                    # 34
#XO4+      0.80663   0.26523  -0.17334                    # 35
#XH*5+     0.90488   0.20967  -0.21618                    # 36
#XLP1+     0.59431   0.31702  -0.17299                    # 37
#XLP1-     0.58321   0.29924  -0.13592                    # 38
#XLP2+     0.53445   0.37239  -0.12199                    # 39
#XLP2-     0.52517   0.35752  -0.09097                    # 40
#XLP3+     0.43379   0.25538  -0.16845                    # 41
#XLP3-     0.45456   0.28866  -0.23783                    # 42
#XLP4+     0.95989   0.28699  -0.21533                    # 43
#XLP4-     0.92845   0.23663  -0.11031                    # 44
#END
```

S13. Optimized crystal structure coordinates for nitroformamidine – nitric acid (cocrystal form).

```
data_NO2F_HNO3_1
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.28189E+01 E(coul)=-2.29361E+01 E(vdW)=-1.98828E+01 Density= 1.94841
;
_cell_length_a   11.544
_cell_length_b    8.538
_cell_length_c    4.978
_cell_angle_alpha   142.52
_cell_angle_beta     99.51
_cell_angle_gamma    65.44
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.60097   0.21461   0.43852                    #  1
N'2       0.47729   0.29847   0.49691                    #  2
N3        0.67303   0.29686   0.41786                    #  3
H*4       0.62519   0.44330   0.45207                    #  4
H*5       0.77217   0.21279   0.36934                    #  5
N6        0.69230  -0.01188   0.37863                    #  6
O7        0.81151  -0.08313   0.32333                    #  7
O8        0.63795  -0.10211   0.39134                    #  8
H*9       0.44939   0.20017   0.49813                    #  9
#XC1      0.59226   0.29238   0.44995                    # 10
#XN'2     0.47170   0.33105   0.50248                    # 11
#XN3      0.68906   0.29220   0.41093                    # 12
```

```
#XH*4      0.62779   0.45763   0.45248                    # 13
#XH*5      0.75264   0.25232   0.38124                    # 14
#XN6       0.71509  -0.06001   0.36454                    # 15
#XO7       0.77476  -0.09073   0.33736                    # 16
#XO8       0.67202  -0.09657   0.37817                    # 17
#XH*9      0.42586   0.22366   0.51001                    # 18
N1+       0.10769   0.58054   0.87783                    # 19
O2+       0.13799   0.66336   0.80179                    # 20
O3+       0.07975   0.68918   1.23744                    # 21
O4+       0.10456   0.31392   0.48180                    # 22
H*5+      0.07882   0.27873   0.60139                    # 23
#XN1+      0.11102   0.66411   0.98600                    # 24
#XO2+      0.13631   0.53524   0.61272                    # 25
#XO3+      0.08195   0.54764   1.00098                    # 26
#XO4+      0.09858   0.39813   0.65420                    # 27
#XH*5+     0.08124   0.28123   0.58885                    # 28
#XLP1+     0.08913   0.63397   0.94387                    # 29
#XLP1-     0.12522   0.59275   0.92143                    # 30
#XLP2+     0.11120   0.71362   0.94218                    # 31
#XLP2-     0.14140   0.67914   0.92341                    # 32
#XLP3+     0.12267   0.68223   1.20384                    # 33
#XLP3-     0.05512   0.75936   1.24584                    # 34
#XLP4+     0.05082   0.33361   0.47083                    # 35
#XLP4-     0.15305   0.21686   0.40726                    # 36
#END

data_NO2F_HNO3_2
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.27800E+01 E(coul)=-2.38349E+01 E(vdW)=-1.89451E+01 Density= 1.88555
;
_cell_length_a    6.225
_cell_length_b   19.408
_cell_length_c    4.435
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 212121'
_symmetry_Int_Tables_number  19
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2+x,1/2-y,-z
  3 -x,1/2+y,1/2-z
  4 1/2-x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

```
C1       -0.41727  -0.15442  -0.55770                    #  1
N'2      -0.46813  -0.11019  -0.36170                    #  2
N3       -0.21845  -0.17507  -0.63965                    #  3
H*4       -0.09103  -0.15351  -0.53579                    #  4
H*5       -0.19942  -0.21118  -0.80091                    #  5
N6       -0.59205  -0.19350  -0.74291                    #  6
O7       -0.53067  -0.23576  -0.92948                    #  7
O8       -0.77838  -0.17903  -0.68805                    #  8
H*9       -0.63086  -0.10478  -0.34631                    #  9
#XC1      -0.32811  -0.14850  -0.52622                    # 10
#XN'2     -0.43328  -0.10706  -0.34575                    # 11
#XN3      -0.20386  -0.18056  -0.66352                    # 12
#XH*4      -0.06920  -0.15381  -0.53595                    # 13
#XH*5      -0.17355  -0.20317  -0.76349                    # 14
#XN6      -0.62484  -0.20293  -0.78707                    # 15
#XO7      -0.58773  -0.22389  -0.87925                    # 16
#XO8      -0.72741  -0.19009  -0.73500                    # 17
#XH*9      -0.63080  -0.09607  -0.30717                    # 18
N1+      -0.01376   0.44286   0.53210                    # 19
O2+      -0.13068   0.46389   0.33767                    # 20
O3+      -0.05227   0.40727   0.75083                    # 21
O4+       0.20241   0.46329   0.49709                    # 22
H*5+      0.27392   0.44234   0.66973                    # 23
#XN1+     -0.08552   0.43865   0.52660                    # 24
#XO2+     -0.02650   0.47354   0.32212                    # 25
#XO3+      0.05593   0.42172   0.70519                    # 26
#XO4+      0.14596   0.45033   0.55694                    # 27
#XH*5+     0.26782   0.44439   0.65329                    # 28
#XLP1+    -0.03343   0.43156   0.51978                    # 29
#XLP1-    -0.04427   0.44746   0.56557                    # 30
#XLP2+    -0.13243   0.44344   0.40739                    # 31
#XLP2-    -0.14150   0.45674   0.44569                    # 32
#XLP3+    -0.10295   0.42792   0.73639                    # 33
#XLP3-    -0.08266   0.39816   0.65070                    # 34
#XLP4+     0.25281   0.44171   0.44233                    # 35
#XLP4-     0.22210   0.48675   0.57203                    # 36
#END

data_NO2F_HNO3_3
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.27716E+01 E(coul)=-2.28638E+01 E(vdW)=-1.99077E+01 Density= 1.94836
;
_cell_length_a   10.028
_cell_length_b    4.978
_cell_length_c    5.499
_cell_angle_alpha   109.14
_cell_angle_beta     91.28
_cell_angle_gamma    89.29
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
```

```
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       -0.10092  -0.27643   0.81518                    #  1
N'2       0.02283  -0.30136   0.77586                    #  2
N3       -0.17302  -0.37977   0.96900                    #  3
H*4       -0.12513  -0.49190   1.06762                    #  4
H*5       -0.27222  -0.34465   0.98370                    #  5
N6       -0.19232  -0.11009   0.67990                    #  6
O7       -0.31160  -0.09467   0.72736                    #  7
O8       -0.13796  -0.00679   0.53574                    #  8
H*9       0.05073  -0.20160   0.64995                    #  9
#XC1      -0.09221  -0.34280   0.88417                    # 10
#XN'2      0.02843  -0.32837   0.80283                    # 11
#XN3      -0.18905  -0.38212   0.98029                    # 12
#XH*4      -0.12773  -0.50585   1.08452                    # 13
#XH*5      -0.25267  -0.37221   1.00373                    # 14
#XN6      -0.21513  -0.07611   0.65452                    # 15
#XO7      -0.27484  -0.07285   0.68322                    # 16
#XO8      -0.17205  -0.02567   0.57517                    # 17
#XH*9       0.07427  -0.21312   0.65000                    # 18
N1+       0.60791   0.20281   0.31213                    # 19
O2+       0.63861   0.36187   0.19966                    # 20
O3+       0.57988  -0.04806   0.23072                    # 21
O4+       0.60437   0.33178   0.58196                    # 22
H*5+      0.57834   0.17688   0.64232                    # 23
#XN1+      0.61140   0.17836   0.22525                    # 24
#XO2+      0.63672   0.42261   0.32950                    # 25
#XO3+      0.58189   0.04664   0.37019                    # 26
#XO4+      0.59845   0.24372   0.50355                    # 27
#XH*5+      0.58079   0.19193   0.63745                    # 28
#XLP1+      0.62547   0.17136   0.28241                    # 29
#XLP1-      0.58941   0.19035   0.27718                    # 30
#XLP2+      0.64195   0.25596   0.18023                    # 31
#XLP2-      0.61178   0.27185   0.17586                    # 32
#XLP3+      0.55541   0.01400   0.18525                    # 33
#XLP3-      0.62290  -0.02155   0.19504                    # 34
#XLP4+      0.65274   0.30888   0.63064                    # 35
#XLP4-      0.55059   0.36269   0.61583                    # 36
#END

data_NO2F_HNO3_4
_chemical_name_systematic
;RAS NH3 PVDZ
```

```
E(total)=-4.26339E+01 E(coul)=-2.35338E+01 E(vdW)=-1.91002E+01 Density= 1.91962
;
_cell_length_a    6.397
_cell_length_b    6.567
_cell_length_c   12.528
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P NA21  '
_symmetry_Int_Tables_number  33
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,1/2+z
  3 1/2+x,1/2-y,z
  4 -x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.98546   0.43141   0.72944                    #  1
N'2       0.98895   0.24125   0.71502                    #  2
N3        0.91611   0.53464   0.81572                    #  3
H*4       0.85893   0.45451   0.87784                    #  4
H*5       0.92196   0.68805   0.81728                    #  5
N6        1.06737   0.58133   0.64237                    #  6
O7        1.05909   0.76407   0.66197                    #  7
O8        1.13415   0.50511   0.56056                    #  8
H*9       1.04992   0.20512   0.64215                    #  9
#XC1      0.94880   0.41388   0.77111                    # 10
#XN'2     0.97432   0.23099   0.73146                    # 11
#XN3      0.91247   0.55892   0.82127                    # 12
#XH*4     0.85059   0.45757   0.88770                    # 13
#XH*5     0.90902   0.65649   0.83061                    # 14
#XN6      1.08351   0.61826   0.62562                    # 15
#XO7      1.07682   0.70945   0.63837                    # 16
#XO8      1.11849   0.55585   0.58155                    # 17
#XH*9     1.04671   0.16851   0.64388                    # 18
N1+       0.32362   0.47452  -0.04953                    # 19
O2+       0.30438   0.58837   0.02474                    # 20
O3+       0.24223   0.31077  -0.06702                    # 21
O4+       0.46390   0.54478  -0.12831                    # 22
H*5+      0.46141   0.43691  -0.18170                    # 23
#XN1+     0.28160   0.46339  -0.02084                    # 24
#XO2+     0.37164   0.62129  -0.01343                    # 25
#XO3+     0.31990   0.36594  -0.10228                    # 26
#XO4+     0.41381   0.49034  -0.11526                    # 27
#XH*5+    0.46208   0.44733  -0.17690                    # 28
#XLP1+    0.28350   0.47490  -0.04839                    # 29
#XLP1-    0.32773   0.44857  -0.03431                    # 30
```

```
#XLP2+     0.25849   0.53482   0.00810                    # 31
#XLP2-     0.29549   0.51280   0.01988                    # 32
#XLP3+     0.27425   0.31840  -0.02961                    # 33
#XLP3-     0.19150   0.36767  -0.05595                    # 34
#XLP4+     0.41983   0.58223  -0.16336                    # 35
#XLP4-     0.54509   0.50766  -0.12348                    # 36
#END

data_NO2F_HNO3_5
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.25882E+01 E(coul)=-2.24709E+01 E(vdW)=-2.01173E+01 Density= 1.95940
;
_cell_length_a    8.541
_cell_length_b    5.980
_cell_length_c   20.199
_cell_angle_alpha    90.00
_cell_angle_beta     88.14
_cell_angle_gamma    90.00
_cell_formula_units_Z  8
_symmetry_space_group_name_H-M 'C 2/C   '
_symmetry_Int_Tables_number  15
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,y,1/2-z
  3 -x,-y,-z
  4 x,-y,1/2+z
  5 1/2+x,1/2+y,z
  6 1/2-x,1/2+y,1/2-z
  7 1/2-x,1/2-y,-z
  8 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.20417   0.54059   0.19974                   #  1
N'2       0.21180   0.53861   0.26203                   #  2
N3        0.07479   0.54272   0.16303                   #  3
H*4      -0.03089   0.54280   0.18676                    #  4
H*5       0.08473   0.54418   0.11315                    #  5
N6        0.35534   0.54084   0.15427                   #  6
O7        0.33886   0.54282   0.09421                   #  7
O8        0.47978   0.53902   0.18205                   #  8
H*9       0.32521   0.53730   0.27646                    #  9
#XC1      0.13622   0.54099   0.20390                     # 10
#XN'2     0.18471   0.53874   0.26476                     # 11
#XN3      0.06789   0.54302   0.15494                     # 12
#XH*4    -0.04638   0.54296   0.18540                      # 13
#XH*5     0.06089   0.54406   0.12291                     # 14
```

```
#XN6       0.38507   0.54096   0.14290                    # 15
#XO7       0.37210   0.54199   0.11281                    # 16
#XO8       0.45039   0.53978   0.16480                    # 17
#XH*9      0.31948   0.53698   0.28828                    # 18
N1+       0.19313  -0.01017   0.55355                    # 19
O2+       0.32607  -0.03080   0.57002                    # 20
O3+       0.12005   0.15646   0.53942                    # 21
O4+       0.11036  -0.21398   0.55038                    # 22
H*5+      0.00685  -0.16842   0.53659                    # 23
#XN1+      0.22768   0.04698   0.55578                    # 24
#XO2+      0.28563  -0.12821   0.56840                    # 25
#XO3+      0.09024   0.03721   0.53978                    # 26
#XO4+      0.11102  -0.12966   0.54770                    # 27
#XH*5+     0.01639  -0.17336   0.53789                    # 28
#XLP1+     0.20658   0.01418   0.54456                    # 29
#XLP1-     0.19350   0.02076   0.56238                    # 30
#XLP2+     0.29764   0.02625   0.55658                    # 31
#XLP2-     0.28669   0.03175   0.57149                    # 32
#XLP3+     0.14971   0.16167   0.56110                    # 33
#XLP3-     0.17420   0.14935   0.52775                    # 34
#XLP4+     0.10897  -0.24667   0.52354                    # 35
#XLP4-     0.07189  -0.22803   0.57402                    # 36
#END
```

S14. Optimized crystal structure coordinates for formamidinium dinitramide (ionic form).

```
data_HF_DN_1
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.60080E+02 E(coul)=-1.43197E+02 E(vdW)=-1.68826E+01 Density= 1.85383
;
_cell_length_a   12.051
_cell_length_b   13.164
_cell_length_c    3.450
_cell_angle_alpha    90.00
_cell_angle_beta     98.40
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

```
C1        0.21398   0.03970   0.91161                    #  1
N2        0.22276   0.12873   0.74580                    #  2
H*3       0.15296   0.17042   0.65727                    #  3
H*4       0.29749   0.15864   0.70067                    #  4
N5        0.29868  -0.02055   1.03718                    #  5
H*6       0.28445  -0.08811   1.16189                    #  6
H*7       0.37949  -0.00259   1.01538                    #  7
H8        0.13008   0.01388   0.94772                    #  8
#XC1      0.21590   0.04029   0.91078                    #  9
#XN2      0.21749   0.12994   0.74275                    # 10
#XH*3     0.13526   0.18505   0.62718                    # 11
#XH*4     0.30835   0.16543   0.68953                    # 12
#XN5      0.29591  -0.02424   1.04370                    # 13
#XH*6     0.28441  -0.10820   1.19960                    # 14
#XH*7     0.39338  -0.00176   1.01587                    # 15
#XH8      0.13649   0.01585   0.94496                    # 16
N'1+     -0.08678   0.29009   0.42575                    # 17
N2+       0.01417   0.33709   0.40378                    # 18
O3+       0.00457   0.41892   0.22072                    # 19
O4+       0.10487   0.30597   0.57820                    # 20
N5+      -0.07929   0.18729   0.49831                    # 21
O6+      -0.00407   0.13303   0.40130                    # 22
O7+      -0.16082   0.15235   0.63886                    # 23
#XN'1+    -0.08670   0.29005   0.42579                   # 24
#XN2+      0.01437   0.33834   0.40444                   # 25
#XO3+      0.01086   0.41223   0.22309                   # 26
#XO4+      0.10809   0.31611   0.56375                   # 27
#XN5+     -0.08037   0.18649   0.49724                   # 28
#XO6+     -0.01195   0.12529   0.41357                   # 29
#XO7+     -0.15126   0.15088   0.64388                   # 30
#XLP1+    -0.06665   0.30226   0.77334                   # 31
#XLP1-    -0.08990   0.26916   0.08610                   # 32
#XLP2+     0.00082   0.37806   0.64757                   # 33
#XLP2-     0.03881   0.31946   0.09951                   # 34
#XLP5+    -0.04819   0.17624   0.82859                   # 35
#XLP5-    -0.12637   0.17741   0.22633                   # 36
#END

data_HF_DN_2
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.60063E+02 E(coul)=-1.42888E+02 E(vdW)=-1.71749E+01 Density= 1.90013
;
_cell_length_a   14.331
_cell_length_b   11.932
_cell_length_c    3.426
_cell_angle_alpha    90.00
_cell_angle_beta    115.61
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
```

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_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.04700   0.28534   0.17198                    #  1
N2       -0.01222   0.20092   0.16969                    #  2
H*3       -0.08092   0.21586   0.17821                    #  3
H*4        0.00767   0.11965   0.15960                    #  4
N5        0.13733   0.27567   0.16176                    #  5
H*6        0.17808   0.34532   0.16448                    #  6
H*7        0.16919   0.20038   0.15104                    #  7
H8        0.01909   0.36980   0.18320                    #  8
#XC1       0.04764   0.28341   0.17172                     #  9
#XN2      -0.01601   0.20374   0.17036                     # 10
#XH*3      -0.10127   0.21609   0.18032                     # 11
#XH*4       0.00880   0.10570   0.15811                     # 12
#XN5       0.13845   0.28095   0.16216                     # 13
#XH*6       0.19252   0.36294   0.16474                     # 14
#XH*7       0.17629   0.18942   0.14922                     # 15
#XH8       0.02122   0.36335   0.18234                     # 16
N'1+     -0.28742   0.41825   0.86898                    # 17
N2+      -0.33380   0.52012   0.71432                    # 18
O3+      -0.41758   0.51240   0.38515                    # 19
O4+      -0.30045   0.60990   0.90481                    # 20
N5+      -0.18249   0.42365   1.12565                    # 21
O6+      -0.12626   0.49800   1.09125                    # 22
O7+      -0.14791   0.34122   1.36909                    # 23
#XN'1+     -0.28737   0.41833   0.86905                     # 24
#XN2+      -0.33507   0.52034   0.71262                     # 25
#XO3+      -0.41067   0.51855   0.39677                     # 26
#XO4+      -0.31075   0.61334   0.87030                     # 27
#XN5+      -0.18169   0.42255   1.12652                     # 28
#XO6+      -0.11847   0.48996   1.12138                     # 29
#XO7+      -0.14626   0.35074   1.37237                     # 30
#XLP1+     -0.29894   0.43798   1.18854                     # 31
#XLP1-     -0.26671   0.41533   0.56541                     # 32
#XLP2+     -0.37533   0.50712   0.89229                     # 33
#XLP2-     -0.31596   0.54496   0.42758                     # 34
#XLP5+     -0.17023   0.45395   1.46483                     # 35
#XLP5-     -0.17358   0.37687   0.89083                     # 36
#END

data_HF_DN_3
_chemical_name_systematic
```

```
;RAS NNO22_C2_PVDZ

E(total)=-1.59436E+02 E(coul)=-1.46324E+02 E(vdW)=-1.31127E+01 Density= 1.73657
;
_cell_length_a   13.745
_cell_length_b    8.248
_cell_length_c    7.133
_cell_angle_alpha    97.76
_cell_angle_beta    152.45
_cell_angle_gamma   107.59
_cell_formula_units_Z  1
_symmetry_space_group_name_H-M 'P 1     '
_symmetry_Int_Tables_number   1
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.04519   0.22145   0.50349                          #  1
N2         0.20689   0.19759   0.84832                          #  2
H*3        0.06255   0.05743   0.70588                          #  3
H*4        0.47493   0.31483   1.25932                          #  4
N5         0.20564   0.39578   0.64283                          #  5
H*6        0.06039   0.40067   0.35001                          #  6
H*7        0.47358   0.52889   1.03739                          #  7
H8        -0.24393   0.08640   0.06894                          #  8
#XC1        0.05181   0.22454   0.51343                          #  9
#XN2        0.19306   0.18786   0.83087                          # 10
#XH*3       0.03214   0.02010   0.68387                          # 11
#XH*4       0.51759   0.33079   1.32750                          # 12
#XN5        0.19177   0.39256   0.61863                          # 13
#XH*6       0.02969   0.40945   0.28019                          # 14
#XH*7       0.51619   0.55276   1.09736                          # 15
#XH8       -0.22185   0.09671   0.10213                          # 16
N'1+      -0.57346   0.17711  -0.16511                          # 17
N2+       -0.17520   0.36570   0.62118                          # 18
O3+       -0.07357   0.47136   0.97812                          # 19
O4+        0.02868   0.39403   0.89079                          # 20
N5+       -0.56777   0.18969  -0.34619                          # 21
O6+       -0.15359   0.46915   0.31017                          # 22
O7+       -1.00884  -0.08501  -1.21170                          # 23
#XN'1+     -0.57316   0.17726  -0.16466                          # 24
#XN2+      -0.17559   0.36461   0.62249                          # 25
#XO3+      -0.04810   0.48587   1.01103                          # 26
#XO4+       0.05074   0.40772   0.94998                          # 27
#XN5+      -0.57067   0.18914  -0.35243                          # 28
#XO6+      -0.19300   0.44682   0.22499                          # 29
#XO7+      -0.97532  -0.07014  -1.15622                          # 30
#XLP1+     -0.83378  -0.13217  -0.67443                          # 31
```

```
#XLP1-     -0.24980   0.51794   0.43912                                  # 32
#XLP2+     -0.48057   0.07299   0.10329                                   # 33
#XLP2-      0.22246   0.72425   1.35401                                  # 34
#XLP5+     -0.75780  -0.06547  -0.76796                                   # 35
#XLP5-     -0.48749   0.37030  -0.16555                                  # 36
#END

data_HF_DN_4
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.59208E+02 E(coul)=-1.43782E+02 E(vdW)=-1.54262E+01 Density= 1.81540
;
_cell_length_a    8.437
_cell_length_b    7.145
_cell_length_c    7.572
_cell_angle_alpha    92.42
_cell_angle_beta     56.16
_cell_angle_gamma   126.22
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.11807  -0.25018   0.25010                                 #  1
N2         0.27136  -0.06164   0.27621                                 #  2
H*3        0.26590   0.07617   0.29545                                  #  3
H*4        0.39787  -0.04638   0.27817                                  #  4
N5         0.10905  -0.43851   0.22383                                 #  5
H*6       -0.01519  -0.57650   0.20474                                  #  6
H*7        0.22257  -0.45342   0.22159                                  #  7
H8        -0.01141  -0.25036   0.25026                                 #  8
#XC1        0.12103  -0.25017   0.25010                                  #  9
#XN2        0.26782  -0.05546   0.27708                                  # 10
#XH*3       0.27110   0.11999   0.30156                                   # 11
#XH*4       0.42020  -0.03884   0.27919                                   # 12
#XN5        0.10018  -0.44470   0.22297                                  # 13
#XH*6      -0.04775  -0.62036   0.19866                                   # 14
#XH*7       0.23842  -0.46091   0.22052                                   # 15
#XH8       -0.00153  -0.25035   0.25024                                  # 16
N'1+       0.51718  -0.25029   0.25002                                  # 17
N2+        0.67910  -0.06817   0.28453                                  # 18
O3+        0.72783   0.13396   0.24107                                  # 19
O4+        0.75061  -0.10898   0.37038                                  # 20
N5+        0.53164  -0.43217   0.21547                                  # 21
```

```
O6+       0.73000  -0.39101   0.12956                                  # 22
O7+       0.33469  -0.63450   0.25896                                  # 23
#XN'1+     0.51731  -0.25029   0.25002                                   # 24
#XN2+      0.67860  -0.06641   0.28585                                   # 25
#XO3+      0.73969   0.12907   0.23820                                  # 26
#XO4+      0.75966  -0.08354   0.37015                                   # 27
#XN5+      0.53070  -0.43393   0.21415                                   # 28
#XO6+      0.71338  -0.41646   0.12979                                   # 29
#XO7+      0.34859  -0.62957   0.26183                                   # 30
#XLP1+     0.36208  -0.38111   0.45706                                    # 31
#XLP1-     0.69993  -0.11943   0.04297                                   # 32
#XLP2+     0.51169  -0.13879   0.45054                                    # 33
#XLP2-     0.88824   0.07816   0.10313                                  # 34
#XLP5+     0.41316  -0.57839   0.39685                                    # 35
#XLP5-     0.60076  -0.36167   0.04948                                   # 36
#END

data_HF_DN_5
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.58932E+02 E(coul)=-1.41474E+02 E(vdW)=-1.74575E+01 Density= 1.88248
;
_cell_length_a    3.340
_cell_length_b   13.566
_cell_length_c   11.874
_cell_angle_alpha    90.00
_cell_angle_beta     82.34
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.03439   0.54301   0.21554                                 #  1
N2       -0.12156   0.48529   0.29902                                 #  2
H*3       -0.20370   0.41548   0.28212                                  #  3
H*4       -0.16511   0.50743   0.38144                                  #  4
N5        0.15111   0.63454   0.22770                                 #  5
H*6        0.26852   0.67396   0.15862                                  #  6
H*7        0.12939   0.66863   0.30441                                  #  7
H8        0.06961   0.51268   0.12970                                 #  8
#XC1       0.03359   0.54371   0.21750                                   #  9
```

```
#XN2      -0.12435   0.48138   0.29608                    # 10
#XH*3     -0.23170   0.39491   0.28135                    # 11
#XH*4     -0.17574   0.50893   0.39552                    # 12
#XN5       0.15728   0.63554   0.22242                    # 13
#XH*6      0.30397   0.68812   0.14125                    # 14
#XH*7      0.12964   0.67608   0.31565                    # 15
#XH8       0.06692   0.51500   0.13625                    # 16
N'1+      0.39663   0.28325   0.58090                     # 17
N2+       0.41790   0.33384   0.47977                     # 18
O3+       0.25510   0.41656   0.48924                     # 19
O4+       0.61092   0.30406   0.38997                     # 20
N5+       0.44041   0.18268   0.56964                     # 21
O6+       0.34692   0.13598   0.48746                     # 22
O7+       0.54855   0.14196   0.65462                     # 23
#XN'1+     0.39668   0.28321   0.58082                    # 24
#XN2+      0.41901   0.33504   0.47965                    # 25
#XO3+      0.25723   0.41034   0.48253                    # 26
#XO4+      0.60036   0.31433   0.38686                    # 27
#XN5+      0.43877   0.18188   0.57068                    # 28
#XO6+      0.35469   0.12786   0.49540                    # 29
#XO7+      0.55592   0.14088   0.64491                    # 30
#XLP1+     0.75821   0.28808   0.56991                    # 31
#XLP1-     0.04525   0.27058   0.57427                    # 32
#XLP2+     0.67368   0.36727   0.50183                    # 33
#XLP2-     0.11133   0.32484   0.44587                    # 34
#XLP5+     0.78042   0.16599   0.54576                    # 35
#XLP5-     0.14839   0.17710   0.61021                    # 36
#END
```

S15. Optimized crystal structure coordinates for azidoformamidinium dinitramide (ionic form).

```
data_N3F_DN_1
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.53196E+02 E(coul)=-1.37673E+02 E(vdW)=-1.55228E+01 Density= 1.71085
;
_cell_length_a    8.672
_cell_length_b   12.267
_cell_length_c    7.526
_cell_angle_alpha    90.00
_cell_angle_beta    111.29
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
```

```
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       -0.09151   0.49752  -0.27555                    #  1
N2       -0.22712   0.44628  -0.27550                    #  2
H*3       -0.34089   0.48024  -0.33272                    #  3
H*4       -0.22049   0.37107  -0.21768                    #  4
N5        0.05747   0.45251  -0.20022                    #  5
H*6       0.15768   0.49399  -0.20295                    #  6
H*7       0.07469   0.37766  -0.13968                    #  7
N'8      -0.09156   0.59926  -0.35127                    #  8
N9       -0.22930   0.64700  -0.42548                    #  9
N'10     -0.34023   0.70055  -0.49647                    # 10
#XC1      -0.08575   0.49304  -0.27060                    # 11
#XN2      -0.22995   0.45199  -0.28054                    # 12
#XH*3     -0.38098   0.48236  -0.34555                    # 13
#XH*4     -0.22454   0.35164  -0.20435                    # 14
#XN5       0.05767   0.45098  -0.19903                    # 15
#XH*6      0.19044   0.49770  -0.19651                    # 16
#XH*7      0.09114   0.35977  -0.12175                    # 17
#XN'8     -0.09439   0.60713  -0.35792                    # 18
#XN9      -0.23561   0.65671  -0.43447                    # 19
#XN'10    -0.34676   0.69011  -0.49054                    # 20
N'1+     -0.10556   0.12667   0.09731                    # 21
N2+       -0.09782   0.21131  -0.01931                    # 22
O3+       -0.23184   0.22989  -0.15133                    # 23
O4+        0.02589   0.26967   0.01331                    # 24
N5+        0.04469   0.07937   0.19898                    # 25
O6+        0.16269   0.07812   0.14347                    # 26
O7+        0.04595   0.02941   0.34356                    # 27
#XN'1+    -0.10544   0.12670   0.09730                    # 28
#XN2+     -0.09929   0.21226  -0.02010                    # 29
#XO3+     -0.21811   0.22991  -0.14989                    # 30
#XO4+      0.01325   0.27568  -0.00268                    # 31
#XN5+      0.04487   0.07811   0.19988                    # 32
#XO6+      0.16855   0.07051   0.16010                    # 33
#XO7+      0.05529   0.03484   0.33993                    # 34
#XLP1+    -0.07462   0.19275   0.22284                    # 35
#XLP1-    -0.11172   0.06645  -0.03057                    # 36
#XLP2+    -0.13949   0.26088   0.06449                    # 37
#XLP2-    -0.08502   0.17418  -0.15439                    # 38
#XLP5+     0.11308   0.13568   0.32637                    # 39
#XLP5-    -0.00168   0.00899   0.12350                    # 40
#END

data_N3F_DN_2
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.53116E+02 E(coul)=-1.37910E+02 E(vdW)=-1.52066E+01 Density= 1.74241
```

```
;
_cell_length_a   19.427
_cell_length_b    6.443
_cell_length_c    8.014
_cell_angle_alpha    90.00
_cell_angle_beta    133.10
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.58516   0.22419  -0.32398                                  #  1
N2        0.67658   0.21605  -0.21076                                  #  2
H*3       0.70037   0.24493  -0.28810                                   #  3
H*4       0.72555   0.18040  -0.04227                                   #  4
N5        0.55438   0.18613  -0.22150                                  #  5
H*6       0.48433   0.19382  -0.31328                                   #  6
H*7       0.59871   0.14942  -0.05368                                   #  7
N'8       0.51523   0.27139  -0.55181                                  #  8
N9        0.53947   0.30942  -0.66028                                  #  9
N'10      0.54863   0.34705  -0.78144                                   # 10
#XC1       0.58585   0.22145  -0.31388                                    # 11
#XN2       0.67383   0.21903  -0.22357                                    # 12
#XH*3      0.71553   0.25053  -0.29329                                     # 13
#XH*4      0.74059   0.17185   0.00121                                     # 14
#XN5       0.55534   0.18540  -0.21808                                    # 15
#XH*6      0.46821   0.19176  -0.32121                                     # 16
#XH*7      0.60420   0.13923  -0.01343                                     # 17
#XN'8      0.51099   0.27537  -0.56947                                    # 18
#XN9       0.53542   0.31465  -0.68208                                    # 19
#XN'10     0.55850   0.34296  -0.75815                                     # 20
N'1+      0.13779   0.68784   0.42697                                   # 21
N2+       0.20757   0.72927   0.65723                                   # 22
O3+       0.17964   0.83137   0.73332                                   # 23
O4+       0.28818   0.65669   0.78108                                   # 24
N5+       0.16993   0.64263   0.32223                                   # 25
O6+       0.24525   0.70944   0.39041                                   # 26
O7+       0.11221   0.54371   0.14066                                   # 27
#XN'1+     0.13786   0.68783   0.42707                                     # 28
#XN2+      0.20740   0.72907   0.65902                                     # 29
#XO3+      0.18643   0.83117   0.73662                                     # 30
#XO4+      0.28825   0.66607   0.79826                                     # 31
```

```
#XN5+      0.16926   0.64286   0.31941                    # 32
#XO6+      0.24080   0.70023   0.36783                    # 33
#XO7+      0.12030   0.54335   0.15570                    # 34
#XLP1+     0.14930   0.50801   0.47870                    # 35
#XLP1-     0.14226   0.86708   0.39493                    # 36
#XLP2+     0.18506   0.59872   0.68288                    # 37
#XLP2-     0.23350   0.89697   0.67771                    # 38
#XLP5+     0.19637   0.47300   0.36625                    # 39
#XLP5-     0.13564   0.77528   0.22663                    # 40
#END

data_N3F_DN_3
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.52914E+02 E(coul)=-1.36962E+02 E(vdW)=-1.59521E+01 Density= 1.77272
;
_cell_length_a   10.977
_cell_length_b    9.605
_cell_length_c    6.991
_cell_angle_alpha    90.00
_cell_angle_beta    102.39
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.52526  -0.10789   0.27057                   #  1
N2        0.58498  -0.22283   0.34599                   #  2
H*3       0.54724  -0.31869   0.31737                   #  3
H*4       0.67078  -0.21780   0.43510                   #  4
N5        0.57530   0.01762   0.30870                   #  5
H*6       0.52703   0.10258   0.24864                   #  6
H*7       0.66059   0.03161   0.39628                   #  7
N'8       0.40912  -0.10717   0.14908                   #  8
N9        0.35586  -0.22318   0.10651                   #  9
N'10      0.29574  -0.31648   0.05421                   # 10
#XC1      0.53032  -0.10306   0.27532                   # 11
#XN2      0.57850  -0.22518   0.33947                   # 12
#XH*3     0.54519  -0.35254   0.31904                   # 13
#XH*4     0.69301  -0.22136   0.45874                   # 14
#XN5      0.57704   0.01778   0.31049                   # 15
```

```
#XH*6      0.52250   0.13029   0.24078                    # 16
#XH*7      0.68087   0.04537   0.41592                    # 17
#XN'8      0.40016  -0.10951   0.13998                    # 18
#XN9       0.34484  -0.22843   0.09559                    # 19
#XN'10     0.30770  -0.32208   0.06736                    # 20
N'1+      0.52203   0.47889   0.30207                    # 21
N2+       0.64199   0.43182   0.36992                    # 22
O3+       0.72268   0.52379   0.37571                    # 23
O4+       0.66689   0.31303   0.43540                    # 24
N5+       0.43676   0.37653   0.22964                    # 25
O6+       0.46495   0.26671   0.15718                    # 26
O7+       0.32692   0.41012   0.22769                    # 27
#XN'1+     0.52205   0.47878   0.30206                    # 28
#XN2+      0.64307   0.43271   0.37151                    # 29
#XO3+      0.72200   0.51210   0.37173                    # 30
#XO4+      0.67934   0.32000   0.44073                    # 31
#XN5+      0.43540   0.37686   0.22809                    # 32
#XO6+      0.45101   0.26614   0.15205                    # 33
#XO7+      0.33266   0.39999   0.23101                    # 34
#XLP1+     0.50412   0.45162   0.46114                    # 35
#XLP1-     0.54537   0.48273   0.14228                    # 36
#XLP2+     0.63366   0.46607   0.50636                    # 37
#XLP2-     0.68545   0.41174   0.23584                    # 38
#XLP5+     0.41114   0.31981   0.36138                    # 39
#XLP5-     0.42576   0.42554   0.09575                    # 40
#END

data_N3F_DN_4
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.52428E+02 E(coul)=-1.37162E+02 E(vdW)=-1.52659E+01 Density= 1.76333
;
_cell_length_a    7.516
_cell_length_b    7.964
_cell_length_c    6.474
_cell_angle_alpha   105.09
_cell_angle_beta     86.24
_cell_angle_gamma   104.75
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.21991  -0.05634   0.25908                    #  1
```

```
N2        0.39941   0.01362   0.23946                    #  2
H*3       0.44820   0.13611   0.21082                    #  3
H*4       0.49345  -0.05424   0.25273                    #  4
N5        0.15675  -0.21718   0.29667                    #  5
H*6       0.01931  -0.26587   0.31058                    #  6
H*7       0.24158  -0.29353   0.31204                    #  7
N'8       0.08536   0.02806   0.24295                    #  8
N9        0.13566   0.18187   0.20722                    #  9
N'10      0.15620   0.31824   0.17606                    # 10
#XC1      0.22110  -0.06482   0.26096                    # 11
#XN2      0.39419   0.02070   0.23798                    # 12
#XH*3     0.47842   0.17111   0.20229                    # 13
#XH*4     0.52250  -0.06700   0.25498                    # 14
#XN5      0.15859  -0.21862   0.29695                    # 15
#XH*6    -0.01258  -0.28997   0.31670                    # 16
#XH*7     0.25171  -0.32200   0.31824                    # 17
#XN'8     0.07728   0.03694   0.24112                    # 18
#XN9      0.12802   0.19514   0.20440                    # 19
#XN'10    0.17538   0.31500   0.17638                    # 20
N'1+      0.23913   0.38505   0.70111                    # 21
N2+       0.29848   0.56852   0.73546                    # 22
O3+       0.19401   0.63572   0.65899                    # 23
O4+       0.43346   0.65997   0.84766                    # 24
N5+       0.37503   0.30038   0.71386                    # 25
O6+       0.53875   0.36008   0.67371                    # 26
O7+       0.31544   0.15015   0.75076                    # 27
#XN'1+    0.23928   0.38512   0.70115                    # 28
#XN2+     0.29707   0.56989   0.73620                    # 29
#XO3+     0.20977   0.63837   0.66051                    # 30
#XO4+     0.42516   0.67411   0.84391                    # 31
#XN5+     0.37484   0.29819   0.71273                    # 32
#XO6+     0.53867   0.34170   0.67544                    # 33
#XO7+     0.32819   0.16193   0.75612                    # 34
#XLP1+    0.22504   0.41046   0.89164                    # 35
#XLP1-    0.28384   0.37512   0.51797                    # 36
#XLP2+    0.21488   0.57725   0.86871                    # 37
#XLP2-    0.36922   0.59878   0.58072                    # 38
#XLP5+    0.40462   0.32089   0.89281                    # 39
#XLP5-    0.34983   0.23659   0.55437                    # 40
#END

data_N3F_DN_5
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.52366E+02 E(coul)=-1.37653E+02 E(vdW)=-1.47129E+01 Density= 1.69678
;
_cell_length_a    8.096
_cell_length_b    9.529
_cell_length_c    9.856
_cell_angle_alpha    90.00
_cell_angle_beta     98.45
```

```
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.27631  -0.21928   0.50227                    #  1
N2        0.32508  -0.33150   0.57862                    #  2
H*3       0.28696  -0.42959   0.54979                    #  3
H*4       0.40250  -0.32204   0.66869                    #  4
N5        0.32678  -0.09082   0.54068                    #  5
H*6       0.28702  -0.00809   0.47989                    #  6
H*7       0.40414  -0.07241   0.62920                    #  7
N'8       0.17183  -0.22454   0.37947                    #  8
N9        0.11888  -0.34363   0.33656                    #  9
N'10      0.06073  -0.44031   0.28379                    # 10
#XC1      0.28108  -0.21418   0.50706                    # 11
#XN2      0.31914  -0.33419   0.57203                    # 12
#XH*3     0.28365  -0.46365   0.55152                    # 13
#XH*4     0.42235  -0.32448   0.69259                    # 14
#XN5      0.32835  -0.09057   0.54250                    # 15
#XH*6     0.28415   0.01947   0.47192                    # 16
#XH*7     0.42298  -0.05757   0.64903                    # 17
#XN'8     0.16366  -0.22734   0.37027                    # 18
#XN9      0.10873  -0.34946   0.32552                    # 19
#XN'10    0.07126  -0.44530   0.29708                    # 20
N'1+      0.27411   0.36749   0.55540                    # 21
N2+       0.41369   0.32695   0.64376                    # 22
O3+       0.50056   0.42726   0.69401                    # 23
O4+       0.44251   0.20377   0.67952                    # 24
N5+       0.20905   0.26567   0.46372                    # 25
O6+       0.29423   0.17104   0.42288                    # 26
O7+       0.05955   0.28500   0.41626                    # 27
#XN'1+    0.27416   0.36739   0.55540                    # 28
#XN2+     0.41432   0.32775   0.64526                    # 29
#XO3+     0.50335   0.41619   0.69012                    # 30
#XO4+     0.45550   0.21151   0.68902                    # 31
#XN5+     0.20781   0.26604   0.46224                    # 32
#XO6+     0.27805   0.16942   0.41352                    # 33
#XO7+     0.06765   0.27527   0.41966                    # 34
#XLP1+    0.19367   0.31604   0.63543                    # 35
#XLP1-    0.36623   0.39662   0.47485                    # 36
#XLP2+    0.34342   0.34061   0.72197                    # 37
```

```
#XLP2-      0.52655   0.33147   0.58447                    # 38
#XLP5+      0.13449   0.18799   0.52130                    # 39
#XLP5-      0.23779   0.33135   0.38736                    # 40
#END
```

S16. Optimized crystal structure coordinates for guanidinium dinitramide (ionic form).

```
data_GH_DN_1
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.65604E+02 E(coul)=-1.45512E+02 E(vdW)=-2.00919E+01 Density= 1.89561
;
_cell_length_a    7.731
_cell_length_b   11.786
_cell_length_c    6.581
_cell_angle_alpha    90.00
_cell_angle_beta     76.10
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.25124  -0.11934   0.05129                   #  1
N2        0.10104  -0.12255  -0.01552                   #  2
H*3      -0.01841  -0.10503   0.08178                    #  3
H*4       0.10259  -0.14259  -0.16525                    #  4
N5        0.24521  -0.09255   0.25033                   #  5
H*6       0.35709  -0.08963   0.30405                    #  6
H*7       0.12859  -0.07444   0.35283                    #  7
N8        0.40748  -0.14292  -0.08094                   #  8
H*9       0.41504  -0.16336  -0.23195                    #  9
H*10      0.52254  -0.14098  -0.03372                    # 10
#XN2       0.10230  -0.12252  -0.01496                    # 11
#XH*3     -0.01631  -0.10584   0.07634                    # 12
#XH*4      0.09957  -0.14180  -0.16022                    # 13
#XN5       0.24526  -0.09277   0.24866                   # 14
#XH*6      0.35224  -0.08922   0.30570                    # 15
#XH*7      0.13341  -0.07468   0.35242                    # 16
#XN8       0.40617  -0.14272  -0.07983                   # 17
#XH*9      0.41780  -0.16295  -0.22817                    # 18
#XH*10     0.52075  -0.14153  -0.03832                    # 19
```

```
#XLP2+     0.09856  -0.15158  -0.00023                    # 20
#XLP2-     0.10941  -0.09340  -0.02819                    # 21
#XLP5+     0.23990  -0.12216   0.26041                    # 22
#XLP5-     0.25075  -0.06398   0.23245                    # 23
#XLP8+     0.39899  -0.17154  -0.06437                    # 24
#XLP8-     0.40984  -0.11336  -0.09233                    # 25
N'1+      0.16862   0.11361   0.62756                    # 26
N2+       0.33385   0.12001   0.67110                    # 27
O3+       0.32838   0.11689   0.86169                    # 28
O4+       0.47520   0.11873   0.53429                    # 29
N5+       0.16161   0.15552   0.43443                    # 30
O6+       0.26233   0.23072   0.34237                    # 31
O7+       0.03412   0.11804   0.36953                    # 32
#XN'1+     0.16874   0.11364   0.62744                    # 33
#XN2+      0.33446   0.11919   0.67289                    # 34
#XO3+      0.33679   0.12177   0.84749                    # 35
#XO4+      0.48170   0.11749   0.55382                    # 36
#XN5+      0.15971   0.15594   0.43385                    # 37
#XO6+      0.24904   0.22988   0.32927                    # 38
#XO7+      0.04882   0.12021   0.36188                    # 39
#XLP1+     0.21741   0.02559   0.54134                    # 40
#XLP1-     0.14464   0.20920   0.69031                    # 41
#XLP2+     0.33243   0.03253   0.67508                    # 42
#XLP2-     0.35507   0.21247   0.71822                    # 43
#XLP5+     0.22171   0.08788   0.31043                    # 44
#XLP5-     0.07486   0.21607   0.51380                    # 45
#END

data_GH_DN_2
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.64151E+02 E(coul)=-1.45432E+02 E(vdW)=-1.87195E+01 Density= 1.83904
;
_cell_length_a    7.690
_cell_length_b   12.046
_cell_length_c    6.650
_cell_angle_alpha    90.00
_cell_angle_beta    103.10
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
C1        0.07146   0.62423  -0.92089                    #  1
N2        0.07554   0.60062  -0.72337                    #  2
H*3       0.19177   0.58437  -0.62159                    #  3
H*4      -0.03750   0.59834  -0.67012                    #  4
N5        0.22315   0.62666  -0.98711                    #  5
H*6       0.22308   0.64431  -1.13570                    #  6
H*7       0.34228   0.61092  -0.89051                    #  7
N8       -0.08431   0.64540  -1.05219                    #  8
H*9      -0.20048   0.64400  -1.00538                    #  9
H*10     -0.09041   0.66342  -1.20205                    # 10
#XN2      0.07550   0.60082  -0.72503                    # 11
#XH*3     0.18693   0.58459  -0.62201                    # 12
#XH*4    -0.03263   0.59797  -0.66848                    # 13
#XN5      0.22188   0.62664  -0.98656                    # 14
#XH*6     0.22608   0.64361  -1.13071                    # 15
#XH*7     0.34023   0.61163  -0.89590                    # 16
#XN8     -0.08301   0.64522  -1.05109                    # 17
#XH*9    -0.19864   0.64448  -1.00995                    # 18
#XH*10   -0.09322   0.66308  -1.19829                    # 19
#XLP2+    0.07050   0.57244  -0.73971                    # 20
#XLP2-    0.08042   0.62972  -0.71478                    # 21
#XLP5+    0.21522   0.59797  -0.99828                    # 22
#XLP5-    0.22514   0.65525  -0.97335                    # 23
#XLP8+   -0.08622   0.61635  -1.06208                    # 24
#XLP8-   -0.07630   0.67363  -1.03715                    # 25
N'1+    -0.01476   0.87935   0.39860                    # 26
N2+     -0.02157   0.84183   0.59223                    # 27
O3+     -0.15476   0.87524   0.65171                    # 28
O4+      0.08527   0.77363   0.69027                    # 29
N5+      0.15288   0.87797   0.35766                    # 30
O6+      0.29209   0.88664   0.49322                    # 31
O7+      0.15093   0.87726   0.16988                    # 32
#XN'1+   -0.01464   0.87932   0.39872                    # 33
#XN2+    -0.02345   0.84136   0.59282                    # 34
#XO3+    -0.13993   0.87376   0.65954                    # 35
#XO4+     0.07156   0.77424   0.70298                    # 36
#XN5+     0.15345   0.87875   0.35583                    # 37
#XO6+     0.29890   0.88771   0.47396                    # 38
#XO7+     0.15958   0.87305   0.18435                    # 39
#XLP1+   -0.02814   0.78407   0.34521                    # 40
#XLP1-    0.02384   0.96854   0.47594                    # 41
#XLP2+   -0.10118   0.77827   0.51888                    # 42
#XLP2-    0.02965   0.91222   0.70863                    # 43
#XLP5+    0.18432   0.78759   0.31973                    # 44
#XLP5-    0.14288   0.96321   0.34593                    # 45
#END

data_GH_DN_3
_chemical_name_systematic
;RAS NNO22_C2_PVDZ
```

```
E(total)=-1.63742E+02 E(coul)=-1.44824E+02 E(vdW)=-1.89180E+01 Density= 1.83723
;
_cell_length_a    6.499
_cell_length_b   12.216
_cell_length_c    7.789
_cell_angle_alpha    90.00
_cell_angle_beta     76.21
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'C C     '
_symmetry_Int_Tables_number   9
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 x,-y,1/2+z
  3 1/2+x,1/2+y,z
  4 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.38230  -0.12589  -0.20150                          #  1
N2         0.31400  -0.12048  -0.35021                          #  2
H*3        0.41172  -0.13665  -0.46925                          #  3
H*4        0.16268  -0.10006  -0.34790                          #  4
N5         0.58343  -0.15313  -0.20851                          #  5
H*6        0.63830  -0.15770  -0.09775                          #  6
H*7        0.68642  -0.16994  -0.32477                          #  7
N8         0.24946  -0.10406  -0.04577                          #  8
H*9        0.09688  -0.08332  -0.03749                          #  9
H*10       0.29778  -0.10766   0.06817                          # 10
#XN2       0.31457  -0.12052  -0.34897                          # 11
#XH*3      0.40623  -0.13586  -0.46714                          # 12
#XH*4      0.16774  -0.10082  -0.35093                          # 13
#XN5       0.58174  -0.15290  -0.20845                          # 14
#XH*6      0.63994  -0.15804  -0.10258                          # 15
#XH*7      0.68603  -0.16977  -0.31998                          # 16
#XN8       0.25057  -0.10424  -0.04708                          # 17
#XH*9      0.10072  -0.08376  -0.03477                          # 18
#XH*10     0.29312  -0.10708   0.06642                          # 19
#XLP2+     0.32999  -0.09256  -0.35196                          # 20
#XLP2-     0.30069  -0.14861  -0.34263                          # 21
#XLP5+     0.59414  -0.12457  -0.21304                          # 22
#XLP5-     0.56483  -0.18062  -0.20370                          # 23
#XLP8+     0.26672  -0.07646  -0.05349                          # 24
#XLP8-     0.23741  -0.13251  -0.04416                          # 25
N'1+       0.19787   0.63382  -0.12055                          # 26
N2+        0.39204   0.59119  -0.11427                          # 27
O3+        0.45941   0.62558   0.01260                          # 28
O4+        0.48241   0.51845  -0.21519                          # 29
```

```
N5+       0.15307   0.62947  -0.28448                                  # 30
O6+       0.29121   0.63034  -0.42476                                  # 31
O7+      -0.03981   0.63455  -0.27887                                  # 32
#XN'1+     0.19799   0.63378  -0.12067                                   # 33
#XN2+      0.39261   0.59076  -0.11239                                   # 34
#XO3+      0.46703   0.62351  -0.00201                                   # 35
#XO4+      0.49574   0.51900  -0.20200                                   # 36
#XN5+      0.15127   0.63028  -0.28507                                   # 37
#XO6+      0.27147   0.63180  -0.43118                                   # 38
#XO7+     -0.02562   0.62975  -0.28729                                   # 39
#XLP1+     0.13116   0.54211  -0.09793                                   # 40
#XLP1-     0.28801   0.71815  -0.16789                                   # 41
#XLP2+     0.30988   0.53295  -0.02894                                   # 42
#XLP2-     0.51971   0.65553  -0.17311                                   # 43
#XLP5+     0.10216   0.54098  -0.30666                                   # 44
#XLP5-     0.15200   0.71388  -0.28196                                   # 45
#END

data_GH_DN_4
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.63533E+02 E(coul)=-1.45160E+02 E(vdW)=-1.83735E+01 Density= 1.82234
;
_cell_length_a    6.634
_cell_length_b   12.162
_cell_length_c    7.705
_cell_angle_alpha    90.00
_cell_angle_beta    103.09
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.06667   0.62697   0.86298                                 #  1
N2       -0.13214   0.60561   0.85876                                 #  2
H*3       -0.18516   0.60284   0.97172                                  #  3
H*4       -0.23514   0.59162   0.74248                                  #  4
N5        0.19958   0.64518   1.01880                                 #  5
H*6       0.35043   0.66147   1.02500                                  #  6
H*7       0.15306   0.64319   1.13491                                  #  7
N8        0.13256   0.63012   0.71137                                 #  8
```

```
H*9       0.03474   0.61661   0.59220                    #  9
H*10      0.28209   0.64611   0.71155                    # 10
#XN2      -0.13047   0.60579   0.85879                   # 11
#XH*3     -0.18684   0.60254   0.96686                    # 12
#XH*4     -0.23470   0.59179   0.74732                    # 13
#XN5       0.19847   0.64503   1.01750                   # 14
#XH*6      0.34667   0.66114   1.02781                    # 15
#XH*7      0.15765   0.64363   1.13306                    # 16
#XN8       0.13201   0.63010   0.71264                   # 17
#XH*9      0.04018   0.61724   0.59426                    # 18
#XH*10     0.27706   0.64550   0.70855                    # 19
#XLP2+    -0.11693   0.57750   0.86287                    # 20
#XLP2-    -0.13955   0.63456   0.85481                    # 21
#XLP5+     0.20829   0.61630   1.01978                    # 22
#XLP5-     0.18567   0.67335   1.01172                    # 23
#XLP8+     0.14258   0.60154   0.71837                    # 24
#XLP8-     0.11995   0.65859   0.71031                    # 25
N'1+      0.25411   0.12016   0.05096                    # 26
N2+       0.44823   0.15695   0.04349                    # 27
O3+       0.50709   0.12357  -0.08964                    # 28
O4+       0.54724   0.22446   0.14977                    # 29
N5+       0.21377   0.12183   0.21853                    # 30
O6+       0.35005   0.11318   0.35719                    # 31
O7+       0.02568   0.12288   0.21713                    # 32
#XN'1+     0.25423   0.12019   0.05108                    # 33
#XN2+      0.44882   0.15741   0.04162                    # 34
#XO3+      0.51500   0.12504  -0.07485                    # 35
#XO4+      0.55990   0.22382   0.13604                    # 36
#XN5+      0.21193   0.12106   0.21910                    # 37
#XO6+      0.33078   0.11216   0.36405                    # 38
#XO7+      0.04023   0.12704   0.22572                    # 39
#XLP1+     0.20111   0.21461   0.03755                    # 40
#XLP1-     0.33123   0.03173   0.08948                    # 41
#XLP2+     0.37480   0.21994  -0.03595                    # 42
#XLP2-     0.56463   0.08709   0.09447                    # 43
#XLP5+     0.17641   0.21146   0.24983                    # 44
#XLP5-     0.20151   0.03741   0.20876                    # 45
#END

data_GH_DN_5
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.63159E+02 E(coul)=-1.43762E+02 E(vdW)=-1.93973E+01 Density= 1.86442
;
_cell_length_a   20.670
_cell_length_b    3.411
_cell_length_c    8.394
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
```

```
_symmetry_space_group_name_H-M 'P CA21  '
_symmetry_Int_Tables_number  29
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,y,1/2+z
  3 1/2+x,-y,z
  4 -x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.87524   0.48840   0.46051                    #  1
N2        0.82433   0.38134   0.37231                    #  2
H*3       0.83014   0.25780   0.26382                    #  3
H*4       0.77858   0.42085   0.41158                    #  4
N5        0.93526   0.43260   0.40554                    #  5
H*6       0.97439   0.51134   0.47023                    #  6
H*7       0.94324   0.31006   0.29770                    #  7
N8        0.86611   0.65127   0.60369                    #  8
H*9       0.82118   0.69607   0.64749                    #  9
H*10      0.90389   0.73430   0.67226                    # 10
#XN2      0.82476   0.38224   0.37305                    # 11
#XH*3     0.82889   0.26091   0.26668                    # 12
#XH*4     0.77951   0.41707   0.40818                    # 13
#XN5      0.93476   0.43307   0.40600                    # 14
#XH*6     0.97392   0.50690   0.46641                    # 15
#XH*7     0.94409   0.31415   0.30118                    # 16
#XN8      0.86619   0.64991   0.60249                    # 17
#XH*9     0.82290   0.69739   0.64845                    # 18
#XH*10    0.90211   0.73399   0.67218                    # 19
#XLP2+    0.82503   0.47773   0.35621                    # 20
#XLP2-    0.82564   0.28914   0.39188                    # 21
#XLP5+    0.93378   0.52799   0.38879                    # 22
#XLP5-    0.93439   0.33940   0.42445                    # 23
#XLP8+    0.86599   0.74237   0.58305                    # 24
#XLP8-    0.86660   0.55378   0.61871                    # 25
N'1+      0.13253  -0.96877   0.58748                    # 26
N2+       0.18566  -0.89316   0.49344                    # 27
O3+       0.22890  -0.70556   0.56317                    # 28
O4+       0.19244  -1.02799   0.35755                    # 29
N5+       0.07656  -1.04752   0.50452                    # 30
O6+       0.06543  -0.91750   0.36959                    # 31
O7+       0.03570  -1.23248   0.58353                    # 32
#XN'1+    0.13253  -0.96877   0.58735                    # 33
#XN2+     0.18642  -0.89361   0.49409                    # 34
#XO3+     0.22678  -0.70548   0.55043                    # 35
#XO4+     0.19898  -1.01092   0.36066                    # 36
#XN5+     0.07582  -1.04704   0.50531                    # 37
#XO6+     0.05901  -0.93443   0.37407                    # 38
#XO7+     0.03741  -1.23302   0.57042                    # 39
```

```
#XLP1+     0.14568  -1.30931   0.57330                    # 40
#XLP1-     0.11893  -0.62872   0.57391                    # 41
#XLP2+     0.20599  -1.14255   0.54159                    # 42
#XLP2-     0.18133  -0.57504   0.44737                    # 43
#XLP5+     0.07942  -1.36725   0.45962                    # 44
#XLP5-     0.05781  -0.79637   0.55501                    # 45
#END
```

S17. Optimized crystal structure coordinates for nitroformamidinium dinitramide (ionic form).

```
data_NO2F_DN_1
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.63944E+02 E(coul)=-1.44002E+02 E(vdW)=-1.99422E+01 Density= 1.93869
;
_cell_length_a   10.245
_cell_length_b    8.117
_cell_length_c   11.200
_cell_angle_alpha    90.00
_cell_angle_beta    133.83
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.63686   0.30362  -0.23221                    #  1
N2        0.66164   0.39970  -0.30842                    #  2
H*3       0.68214   0.34575  -0.37663                    #  3
H*4       0.66124   0.52455  -0.30230                    #  4
N5        0.60830   0.34110  -0.13863                    #  5
H*6       0.60181   0.45927  -0.11316                    #  6
H*7       0.59200   0.24673  -0.08970                    #  7
N8        0.64211   0.11824  -0.25630                    #  8
O9        0.61912   0.02849  -0.18559                    #  9
O10       0.66866   0.08291  -0.34328                    # 10
#XC1      0.63686   0.30371  -0.23219                    # 11
#XN2      0.66291   0.38330  -0.31314                    # 12
#XH*3     0.68882   0.36604  -0.39738                    # 13
#XH*4     0.66136   0.54338  -0.30198                    # 14
#XN5      0.60801   0.32299  -0.13840                    # 15
#XH*6     0.60066   0.47669  -0.10877                    # 16
```

```
#XH*7      0.58461   0.25156  -0.06568                    # 17
#XN8       0.64186   0.12725  -0.25513                    # 18
#XO9       0.62231   0.01138  -0.19656                    # 19
#XO10      0.66659   0.06002  -0.33751                    # 20
N'1+      0.29940  -0.22081   0.69301                    # 21
N2+       0.41134  -0.25262   0.85943                    # 22
O3+       0.39457  -0.15209   0.93209                    # 23
O4+       0.50755  -0.37705   0.92761                    # 24
N5+       0.35527  -0.28896   0.62203                    # 25
O6+       0.51579  -0.31745   0.69988                    # 26
O7+       0.23103  -0.30549   0.46917                    # 27
#XN'1+     0.29953  -0.22089   0.69308                    # 28
#XN2+      0.41065  -0.25250   0.86042                    # 29
#XO3+      0.40660  -0.15897   0.93540                    # 30
#XO4+      0.50927  -0.37000   0.94097                    # 31
#XN5+      0.35459  -0.28826   0.62027                    # 32
#XO6+      0.50688  -0.32021   0.68242                    # 33
#XO7+      0.24351  -0.31321   0.47979                    # 34
#XLP1+     0.22843  -0.35034   0.66937                    # 35
#XLP1-     0.39669  -0.10696   0.73162                    # 36
#XLP2+     0.30422  -0.31586   0.82876                    # 37
#XLP2-     0.53470  -0.16572   0.93046                    # 38
#XLP5+     0.31815  -0.42723   0.60005                    # 39
#XLP5-     0.36888  -0.17002   0.59952                    # 40
#END

data_NO2F_DN_2
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.63857E+02 E(coul)=-1.43586E+02 E(vdW)=-2.02710E+01 Density= 1.94551
;
_cell_length_a   10.269
_cell_length_b   16.243
_cell_length_c    8.028
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  8
_symmetry_space_group_name_H-M 'P BCA   '
_symmetry_Int_Tables_number  61
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,z
  3 x,1/2-y,1/2+z
  4 1/2-x,-y,1/2+z
  5 -x,-y,-z
  6 1/2+x,1/2-y,-z
  7 -x,1/2+y,1/2-z
  8 1/2+x,y,1/2-z
loop_
```

```
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       -0.30891   0.88141  -0.19608                    #  1
N2       -0.21186   0.92964  -0.15784                    #  2
H*3      -0.16113   0.95619  -0.25306                    #  3
H*4      -0.18545   0.94152  -0.03829                    #  4
N5       -0.38795   0.84065  -0.09924                    #  5
H*6      -0.38159   0.84239   0.02699                    #  6
H*7      -0.45869   0.80580  -0.15403                    #  7
N8       -0.33391   0.87102  -0.38357                    #  8
O9       -0.42411   0.82619  -0.41962                    #  9
O10      -0.26058   0.90884  -0.47404                    # 10
#XC1      -0.30890   0.88141  -0.19599                   # 11
#XN2      -0.21163   0.92997  -0.17615                   # 12
#XH*3     -0.13621   0.96862  -0.24808                   # 13
#XH*4     -0.18089   0.94361  -0.02066                   # 14
#XN5      -0.39284   0.83839  -0.11584                   # 15
#XH*6     -0.38126   0.84234   0.04603                   # 16
#XH*7     -0.48021   0.79477  -0.13360                   # 17
#XN8      -0.33270   0.87152  -0.37446                   # 18
#XO9      -0.41813   0.82946  -0.44273                   # 19
#XO10     -0.27196   0.90333  -0.49138                   # 20
N'1+      0.47623   0.65411  -0.27499                    # 21
N2+       0.36684   0.69025  -0.20805                    # 22
O3+       0.37845   0.76573  -0.18510                    # 23
O4+       0.26300   0.65303  -0.18655                    # 24
N5+       0.48548   0.57055  -0.24870                    # 25
O6+       0.43609   0.53523  -0.12755                    # 26
O7+       0.55802   0.53492  -0.34999                    # 27
#XN'1+     0.47616   0.65407  -0.27492                   # 28
#XN2+      0.36624   0.69115  -0.20871                   # 29
#XO3+      0.37358   0.76039  -0.17790                   # 30
#XO4+      0.25905   0.66173  -0.18326                   # 31
#XN5+      0.48689   0.57004  -0.24879                   # 32
#XO6+      0.44434   0.52856  -0.13483                   # 33
#XO7+      0.54827   0.53333  -0.34357                   # 34
#XLP1+     0.41057   0.63838  -0.39431                   # 35
#XLP1-     0.52619   0.66241  -0.14105                   # 36
#XLP2+     0.34002   0.70425  -0.32857                   # 37
#XLP2-     0.38403   0.69819  -0.06671                   # 38
#XLP5+     0.41681   0.53824  -0.34211                   # 39
#XLP5-     0.56811   0.58297  -0.18013                   # 40
#END

data_NO2F_DN_3
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.63325E+02 E(coul)=-1.44089E+02 E(vdW)=-1.92360E+01 Density= 1.96266
;
```

```
_cell_length_a    7.468
_cell_length_b   11.524
_cell_length_c    7.712
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 212121'
_symmetry_Int_Tables_number  19
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2+x,1/2-y,-z
  3 -x,1/2+y,1/2-z
  4 1/2-x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.12228  -0.34985   0.52998                          #  1
N2        0.17330  -0.28473   0.65920                          #  2
H*3       0.19226  -0.32348   0.77677                          #  3
H*4       0.19449  -0.19804   0.64699                          #  4
N5        0.08929  -0.32201   0.36918                          #  5
H*6       0.10092  -0.23956   0.32392                          #  6
H*7       0.05030  -0.38648   0.28667                          #  7
N8        0.09724  -0.47887   0.57381                          #  8
O9        0.04979  -0.53971   0.45392                          #  9
O10       0.12780  -0.50509   0.72327                          # 10
#XC1      0.12229  -0.34978   0.52995                          # 11
#XN2      0.17219  -0.29620   0.66750                          # 12
#XH*3     0.20503  -0.30983   0.81204                          # 13
#XH*4     0.19795  -0.18497   0.64618                          # 14
#XN5      0.08574  -0.33456   0.36903                          # 15
#XH*6     0.10236  -0.22739   0.31616                          # 16
#XH*7     0.04092  -0.38266   0.24546                          # 17
#XN8      0.09846  -0.47260   0.57168                          # 18
#XO9      0.05123  -0.55179   0.47295                          # 19
#XO10     0.12096  -0.52084   0.71370                          # 20
N'1+      0.61835   0.39132   0.56803                          # 21
N2+       0.60788   0.50729   0.52632                          # 22
O3+       0.48864   0.56020   0.60692                          # 23
O4+       0.71636   0.55664   0.42993                          # 24
N5+       0.69996   0.32322   0.44445                          # 25
O6+       0.70030   0.34709   0.28795                          # 26
O7+       0.75943   0.23009   0.50274                          # 27
#XN'1+    0.61841   0.39136   0.56790                          # 28
#XN2+     0.60760   0.50833   0.52780                          # 29
#XO3+     0.49417   0.56052   0.59294                          # 30
#XO4+     0.70604   0.56667   0.43708                          # 31
#XN5+     0.69965   0.32178   0.44432                          # 32
```

```
#XO6+      0.70757   0.33501   0.28790                    # 33
#XO7+      0.76429   0.23675   0.49259                    # 34
#XLP1+     0.76523   0.41176   0.62288                    # 35
#XLP1-     0.48263   0.37839   0.48726                    # 36
#XLP2+     0.68962   0.52237   0.63173                    # 37
#XLP2-     0.49155   0.51883   0.42903                    # 38
#XLP5+     0.85284   0.33628   0.45679                    # 39
#XLP5-     0.57858   0.28147   0.43115                    # 40
#END

data_NO2F_DN_4
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.63279E+02 E(coul)=-1.44900E+02 E(vdW)=-1.83790E+01 Density= 1.90103
;
_cell_length_a   11.097
_cell_length_b    8.669
_cell_length_c   11.292
_cell_angle_alpha    90.00
_cell_angle_beta    140.90
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.33948   0.70117   0.75463                   #  1
N2        0.36510   0.65000   0.66671                   #  2
H*3       0.39236   0.72874   0.62246                    #  3
H*4       0.35894   0.53612   0.64114                    #  4
N5        0.30322   0.62566   0.82432                   #  5
H*6       0.29001   0.50901   0.81671                    #  6
H*7       0.28778   0.68761   0.88881                    #  7
N8        0.35425   0.87702   0.77993                   #  8
O9        0.33050   0.92505   0.86165                   #  9
O10       0.38797   0.94766   0.71528                    # 10
#XC1       0.33947   0.70109   0.75461                    # 11
#XN2       0.36738   0.66672   0.66677                    # 12
#XH*3      0.39951   0.72004   0.59997                    # 13
#XH*4      0.35824   0.51922   0.63678                    # 14
#XN5       0.30369   0.64167   0.82897                    # 15
#XH*6      0.28782   0.49152   0.81613                    # 16
```

```
#XH*7      0.27862   0.67248   0.90787                    # 17
#XN8       0.35354   0.86848   0.77870                    # 18
#XO9       0.33515   0.94522   0.85661                    # 19
#XO10      0.38652   0.96543   0.72578                    # 20
N'1+      0.29060   0.80296   0.22193                    # 21
N2+       0.35987   0.70941   0.18608                    # 22
O3+       0.25010   0.69793   0.01601                    # 23
O4+       0.52243   0.65319   0.31105                    # 24
N5+       0.37005   0.77715   0.39228                    # 25
O6+       0.43503   0.65075   0.47311                    # 26
O7+       0.35485   0.88893   0.44932                    # 27
#XN'1+     0.29071   0.80287   0.22203                    # 28
#XN2+      0.35972   0.70986   0.18453                    # 29
#XO3+      0.26011   0.68955   0.02864                    # 30
#XO4+      0.51596   0.64953   0.29381                    # 31
#XN5+      0.36899   0.77767   0.39274                    # 32
#XO6+      0.43513   0.65953   0.48458                    # 33
#XO7+      0.36656   0.87987   0.45634                    # 34
#XLP1+     0.42386   0.88594   0.30375                    # 35
#XLP1-     0.18065   0.70127   0.16120                    # 36
#XLP2+     0.41166   0.80839   0.18638                    # 37
#XLP2-     0.28761   0.59019   0.14035                    # 38
#XLP5+     0.51874   0.83502   0.50715                    # 39
#XLP5-     0.23539   0.74468   0.31703                    # 40
#END

data_NO2F_DN_5
_chemical_name_systematic
;RAS NNO22_C2_PVDZ

E(total)=-1.63225E+02 E(coul)=-1.43051E+02 E(vdW)=-2.01736E+01 Density= 1.94285
;
_cell_length_a    8.169
_cell_length_b    8.340
_cell_length_c   10.623
_cell_angle_alpha    90.00
_cell_angle_beta    112.11
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'C C     '
_symmetry_Int_Tables_number   9
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 x,-y,1/2+z
  3 1/2+x,1/2+y,z
  4 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

```
C1       -0.20623   0.06553  -0.01179                    #  1
N2       -0.28797   0.15774   0.04482                    #  2
H*3       -0.35351   0.10424   0.09856                    #  3
H*4       -0.28861   0.27920   0.03737                    #  4
N5       -0.11432   0.10341  -0.08472                    #  5
H*6       -0.09519   0.21869  -0.10693                    #  6
H*7       -0.06007   0.01244  -0.12035                    #  7
N8       -0.22033  -0.11505   0.01083                    #  8
O9       -0.14446  -0.20120  -0.04168                    #  9
O10       -0.30572  -0.15075   0.07862                    # 10
#XC1      -0.20622   0.06562  -0.01181                    # 11
#XN2      -0.29181   0.14172   0.04882                    # 12
#XH*3     -0.37545   0.12364   0.11411                    # 13
#XH*4     -0.28932   0.29751   0.03671                    # 14
#XN5      -0.11311   0.08582  -0.08450                    # 15
#XH*6     -0.09172   0.23569  -0.11070                    # 16
#XH*7     -0.03622   0.01751  -0.13896                    # 17
#XN8      -0.21965  -0.10628   0.00974                    # 18
#XO9      -0.15454  -0.21801  -0.03286                    # 19
#XO10     -0.29868  -0.17291   0.07468                    # 20
N'1+      0.33341  -0.08986   0.78751                    # 21
N2+       0.17291  -0.02545   0.77521                    # 22
O3+       0.08958  -0.10951   0.82767                    # 23
O4+       0.12295   0.10943   0.72759                    # 24
N5+       0.39931  -0.03411   0.69399                    # 25
O6+       0.30455   0.01487   0.57972                    # 26
O7+       0.56214  -0.05102   0.73045                    # 27
#XN'1+     0.33334  -0.08977   0.78743                    # 28
#XN2+      0.17217  -0.02543   0.77648                    # 29
#XO3+      0.08579  -0.10176   0.81797                    # 30
#XO4+      0.10932   0.10509   0.73324                    # 31
#XN5+      0.40082  -0.03510   0.69358                    # 32
#XO6+      0.32224   0.01406   0.57860                    # 33
#XO7+      0.55211  -0.04122   0.72469                    # 34
#XLP1+     0.39972   0.02519   0.85517                    # 35
#XLP1-     0.25228  -0.18607   0.70325                    # 36
#XLP2+     0.23723   0.02353   0.87030                    # 37
#XLP2-     0.06453  -0.08917   0.68581                    # 38
#XLP5+     0.45907   0.09138   0.72901                    # 39
#XLP5-     0.38771  -0.15004   0.65787                    # 40
#END
```

S18. Optimized crystal structure coordinates for formamidine – dinitramic acid (cocrystal form).

```
data_05695_-4.53068E+01
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.53068E+01 E(coul)=-2.90565E+01 E(vdW)=-1.62503E+01 Density= 1.72948
;
_cell_length_a    7.571
_cell_length_b    6.388
```

```
_cell_length_c    7.724
_cell_angle_alpha    99.02
_cell_angle_beta     68.08
_cell_angle_gamma   122.99
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.29288   0.50298  -0.62210                    #  1
N2        0.30824   0.68492  -0.71132                    #  2
H*3       0.32862   0.67424  -0.84842                    #  3
H*4       0.22804   0.77124  -0.63296                    #  4
N'5       0.21313   0.46921  -0.44367                    #  5
H*6       0.22335   0.33231  -0.40421                    #  6
H7        0.36070   0.39720  -0.71915                    #  7
#XC1       0.26472   0.60693  -0.61145                    #  8
#XN2       0.29085   0.69592  -0.71451                    #  9
#XH*3      0.31701   0.68194  -0.80013                    # 10
#XH*4      0.25750   0.75189  -0.67779                    # 11
#XN'5      0.20963   0.51369  -0.45810                    # 12
#XH*6      0.21791   0.32077  -0.38726                    # 13
#XH7       0.38485   0.36530  -0.73064                    # 14
N1+       0.13100   0.79063  -0.18841                    # 15
N'2+      0.24208   0.82204  -0.05917                    # 16
O3+       0.26634   0.98511   0.04886                    # 17
O4+       0.28767   0.66280  -0.07297                    # 18
N'5+      0.18509   1.01323  -0.27741                    # 19
O6+       0.20526   1.19001  -0.18505                    # 20
O7+       0.19206   0.98356  -0.43912                    # 21
H*8+      0.16716   0.68477  -0.29233                    # 22
#XN1+      0.03996   0.75286  -0.13922                    # 23
#XN'2+     0.17972   0.77571  -0.09797                    # 24
#XO3+      0.30582   0.92712   0.02189                    # 25
#XO4+      0.27531   0.69009  -0.13899                    # 26
#XN'5+     0.13936   0.91111  -0.25253                    # 27
#XO6+      0.23152   1.17638  -0.26265                    # 28
#XO7+      0.20693   0.91950  -0.40086                    # 29
#XH*8+     0.17628   0.67924  -0.30376                    # 30
#XLP1+     0.25781   0.97978  -0.22914                    # 31
#XLP1-     0.14466   0.84377  -0.17326                    # 32
#XLP2+     0.33229   0.87064  -0.03819                    # 33
#XLP2-     0.14688   0.81319  -0.09950                    # 34
#XLP3+     0.18305   0.94610  -0.03385                    # 35
#XLP3-     0.15171   0.71181   0.10640                    # 36
```

```
#XLP4+     0.29531   0.73698  -0.04804                    # 37
#XLP4-     0.22810   0.67441  -0.18340                    # 38
#XLP5+     0.25761   1.12117  -0.32417                    # 39
#XLP5-     0.12222   0.89594  -0.19395                    # 40
#XLP6+     0.15756   1.03160  -0.13145                    # 41
#XLP6-     0.04688   1.06353  -0.29509                    # 42
#XLP7+     0.20557   1.03808  -0.39175                    # 43
#XLP7-     0.18047   0.83420  -0.36580                    # 44
#END

data_09895_-4.52759E+01
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.52759E+01 E(coul)=-2.83817E+01 E(vdW)=-1.68941E+01 Density= 1.77092
;
_cell_length_a    8.929
_cell_length_b    6.026
_cell_length_c   12.646
_cell_angle_alpha    90.00
_cell_angle_beta    123.60
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.03352   0.73315  -0.35552                   #  1
N2       -0.06797   0.74768  -0.48554                   #  2
H*3      -0.17861   0.84437  -0.52896                   #  3
H*4      -0.00347   0.72613  -0.53008                   #  4
N'5       0.19543   0.66069  -0.29316                   #  5
H*6       0.24564   0.65493  -0.19860                   #  6
H7       -0.04028   0.78418  -0.31283                   #  7
#XC1       0.03152   0.72088  -0.41814                   #  8
#XN2      -0.06873   0.76110  -0.49938                   #  9
#XH*3     -0.13937   0.81281  -0.51747                   # 10
#XH*4     -0.04173   0.74386  -0.52709                   # 11
#XN'5      0.17789   0.66399  -0.32461                   # 12
#XH*6      0.26187   0.64843  -0.18735                   # 13
#XH7      -0.04923   0.78241  -0.29119                   # 14
N1+       0.40384  -0.09079   0.10939                   # 15
N'2+      0.58575  -0.11649   0.22156                   # 16
```

```
O3+       0.70674  -0.14633   0.20725                    # 17
O4+       0.59169  -0.09221   0.31953                    # 18
N'5+      0.34570  -0.23466   0.00056                    # 19
O6+       0.44947  -0.27298  -0.02961                    # 20
O7+       0.18896  -0.29047  -0.05125                    # 21
H*8+      0.31709  -0.11450   0.13711                    # 22
#XN1+     0.40770  -0.00583   0.09045                    # 23
#XN'2+    0.51650  -0.07899   0.18673                    # 24
#XO3+     0.69832  -0.15919   0.24799                    # 25
#XO4+     0.52096  -0.12005   0.27015                    # 26
#XN'5+    0.34649  -0.16267   0.03022                    # 27
#XO6+     0.38536  -0.31326  -0.04015                    # 28
#XO7+     0.23293  -0.26184   0.00497                    # 29
#XH*8+    0.31013  -0.12223   0.14056                    # 30
#XLP1+    0.42806  -0.24646   0.08362                    # 31
#XLP1-    0.42625  -0.11157   0.09968                    # 32
#XLP2+    0.65094  -0.17778   0.26534                    # 33
#XLP2-    0.49967  -0.07372   0.14751                    # 34
#XLP3+    0.58411  -0.11617   0.13657                    # 35
#XLP3-    0.70368   0.03833   0.28765                    # 36
#XLP4+    0.62118  -0.11314   0.30034                    # 37
#XLP4-    0.45399  -0.10426   0.22814                    # 38
#XLP5+    0.33639  -0.33263  -0.02426                    # 39
#XLP5-    0.39578  -0.12487   0.05186                    # 40
#XLP6+    0.47676  -0.16901   0.03773                    # 41
#XLP6-    0.26208  -0.17906  -0.11891                    # 42
#XLP7+    0.24313  -0.29924  -0.04771                    # 43
#XLP7-    0.25337  -0.20302   0.04343                    # 44
#END

data_01589_-4.51843E+01
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.51843E+01 E(coul)=-2.86509E+01 E(vdW)=-1.65334E+01 Density= 1.75010
;
_cell_length_a    6.878
_cell_length_b    7.892
_cell_length_c   10.565
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P NA21  '
_symmetry_Int_Tables_number  33
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,1/2+z
  3 1/2+x,1/2-y,z
  4 -x,-y,1/2+z
loop_
```

```
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.10027   0.87584   0.49707                    #  1
N2        0.01805   0.98294   0.58427                    #  2
H*3      -0.01514   1.10247   0.55842                     #  3
H*4      -0.06351   0.92963   0.65339                     #  4
N'5       0.10203   0.71481   0.51218                    #  5
H*6       0.17552   0.65802   0.43995                     #  6
H7        0.16697   0.94320   0.41670                    #  7
#XC1      0.03991   0.88358   0.55993                      #  8
#XN2     -0.00571   0.98813   0.59250                      #  9
#XH*3    -0.00953   1.06115   0.57035                      # 10
#XH*4    -0.04453   0.96541   0.63284                      # 11
#XN'5     0.07728   0.73469   0.53547                     # 12
#XH*6     0.18076   0.64135   0.43647                      # 13
#XH7      0.19868   0.94756   0.39413                      # 14
N1+       0.02472   0.47073   0.22001                     # 15
N'2+      0.16471   0.37310   0.29354                     # 16
O3+       0.26876   0.44692   0.36668                     # 17
O4+       0.14977   0.22135   0.27427                     # 18
N'5+      0.08552   0.63298   0.16731                     # 19
O6+       0.18389   0.72544   0.23139                     # 20
O7+       0.01692   0.65735   0.06248                     # 21
H*8+     -0.01957   0.39632   0.14631                      # 22
#XN1+    -0.03006   0.49119   0.25807                      # 23
#XN'2+    0.09232   0.39475   0.27262                      # 24
#XO3+     0.27069   0.38227   0.34361                      # 25
#XO4+     0.12127   0.27279   0.23442                      # 26
#XN'5+    0.03624   0.57879   0.18322                      # 27
#XO6+     0.16746   0.72108   0.17903                      # 28
#XO7+     0.02626   0.58461   0.08295                      # 29
#XH*8+   -0.01918   0.38917   0.13798                       # 30
#XLP1+    0.14819   0.53899   0.19014                      # 31
#XLP1-    0.05458   0.49714   0.23055                      # 32
#XLP2+    0.25029   0.33890   0.30069                      # 33
#XLP2-    0.07814   0.44795   0.27612                      # 34
#XLP3+    0.16551   0.50355   0.31997                      # 35
#XLP3-    0.13871   0.29925   0.40279                      # 36
#XLP4+    0.18483   0.26522   0.29242                      # 37
#XLP4-    0.06544   0.30907   0.20977                      # 38
#XLP5+    0.14652   0.67943   0.13527                      # 39
#XLP5-    0.04386   0.56043   0.22148                      # 40
#XLP6+    0.13010   0.61978   0.26352                      # 41
#XLP6-   -0.00696   0.77733   0.17056                      # 42
#XLP7+    0.06013   0.67449   0.09361                      # 43
#XLP7-   -0.00074   0.52626   0.10427                      # 44
#END

data_04735_-4.51129E+01
_chemical_name_systematic
```

```
;RAS NH3 PVDZ

E(total)=-4.51129E+01 E(coul)=-2.92054E+01 E(vdW)=-1.59075E+01 Density= 1.70034
;
_cell_length_a   11.597
_cell_length_b    6.497
_cell_length_c    8.114
_cell_angle_alpha    90.00
_cell_angle_beta    105.09
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.62049   0.63894  -0.01211                                  #  1
N2        0.64788   0.46275   0.08336                                  #  2
H*3       0.62644   0.45303   0.19582                                   #  3
H*4       0.65083   0.32979   0.01953                                   #  4
N'5       0.61759   0.64409  -0.17095                                  #  5
H*6       0.59995   0.78963  -0.21754                                   #  6
H7        0.60489   0.77246   0.06299                                  #  7
#XC1       0.63401   0.52046  -0.01228                                    #  8
#XN2       0.64288   0.43521   0.08497                                    #  9
#XH*3      0.63312   0.44864   0.15610                                     # 10
#XH*4      0.64924   0.36284   0.05741                                     # 11
#XN'5      0.62293   0.59618  -0.15453                                     # 12
#XH*6      0.59871   0.79975  -0.23332                                     # 13
#XH7       0.60512   0.82131   0.07172                                     # 14
N1+       0.33452   0.68955   0.35500                                    # 15
N'2+      0.36434   0.63587   0.53558                                    # 16
O3+       0.36586   0.77023   0.63824                                    # 17
O4+       0.37871   0.45113   0.55825                                    # 18
N'5+      0.38372   0.87840   0.30407                                    # 19
O6+       0.38662   1.03016   0.39012                                    # 20
O7+       0.41121   0.85802   0.16985                                    # 21
H*8+      0.36183   0.57060   0.29191                                     # 22
#XN1+      0.28464   0.70909   0.34146                                     # 23
#XN'2+     0.34076   0.63520   0.46442                                     # 24
#XO3+      0.38469   0.68956   0.64197                                     # 25
#XO4+      0.38520   0.49140   0.49241                                     # 26
#XN'5+     0.35449   0.80696   0.30046                                     # 27
#XO6+      0.40995   1.00575   0.34014                                     # 28
```

```
#XO7+      0.40844   0.78241   0.21463                    # 29
#XH*8+     0.36740   0.56008   0.28798                    # 30
#XLP1+     0.40636   0.79346   0.39287                    # 31
#XLP1-     0.34077   0.73116   0.37476                    # 32
#XLP2+     0.40316   0.62171   0.60883                    # 33
#XLP2-     0.32840   0.69376   0.44101                    # 34
#XLP3+     0.34045   0.79422   0.51568                    # 35
#XLP3-     0.29250   0.57464   0.62566                    # 36
#XLP4+     0.38178   0.51648   0.58189                    # 37
#XLP4-     0.37072   0.51108   0.42484                    # 38
#XLP5+     0.42855   0.93951   0.30547                    # 39
#XLP5-     0.33679   0.79873   0.34081                    # 40
#XLP6+     0.34912   0.90268   0.41214                    # 41
#XLP6-     0.32814   1.02080   0.19977                    # 42
#XLP7+     0.41229   0.89843   0.21729                    # 43
#XLP7-     0.38691   0.71378   0.23135                    # 44
#END

data_08361_-4.50169E+01
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.50169E+01 E(coul)=-2.83630E+01 E(vdW)=-1.66540E+01 Density= 1.72766
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_cell_length_a    6.359
_cell_length_b   11.620
_cell_length_c    7.927
_cell_angle_alpha    90.00
_cell_angle_beta     82.71
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.18052   0.62275   0.53754                   #  1
N2        0.00425   0.64536   0.45954                   #  2
H*3       0.00765   0.62812   0.33456                    #  3
H*4      -0.13822   0.64141   0.53255                    #  4
N'5       0.17201   0.61529   0.69948                   #  5
H*6       0.31974   0.60234   0.73295                    #  6
H7        0.32652   0.61506   0.44720                   #  7
#XC1       0.05698   0.63132   0.54913                     #  8
```

```
#XN2      -0.02307   0.63967   0.45688                    #  9
#XH*3     -0.00144   0.63308   0.37866                    # 10
#XH*4     -0.10071   0.64225   0.49135                    # 11
#XN'5      0.12355   0.61914   0.68715                    # 12
#XH*6      0.32889   0.60105   0.74818                    # 13
#XH7       0.37735   0.61731   0.43614                    # 14
N1+       0.69347   0.15730   0.08214                    # 15
N'2+      0.88234   0.11202   0.14549                    # 16
O3+       1.04624   0.11004   0.05111                    # 17
O4+       0.84867   0.08623   0.29557                    # 18
N'5+      0.65494   0.12705  -0.08974                    # 19
O6+       0.80253   0.12616  -0.20099                    # 20
O7+       0.46718   0.11145  -0.09907                    # 21
H*8+      0.56519   0.13038   0.16330                    # 22
#XN1+     0.71266   0.20551   0.07552                    # 23
#XN'2+    0.80884   0.13950   0.14090                    # 24
#XO3+     1.01632   0.08772   0.11292                    # 25
#XO4+     0.77520   0.08794   0.25175                    # 26
#XN'5+    0.64780   0.15014  -0.02569                    # 27
#XO6+     0.71986   0.10732  -0.19375                    # 28
#XO7+     0.50236   0.10598  -0.03050                    # 29
#XH*8+    0.55397   0.12496   0.17002                    # 30
#XLP1+    0.72622   0.09403  -0.01285                    # 31
#XLP1-    0.72591   0.15235   0.04985                    # 32
#XLP2+    0.94491   0.06946   0.15899                    # 33
#XLP2-    0.80428   0.15618   0.09271                    # 34
#XLP3+    0.91763   0.14482   0.01939                    # 35
#XLP3-    1.01931   0.16735   0.22459                    # 36
#XLP4+    0.89461   0.08526   0.24528                    # 37
#XLP4-    0.70642   0.10792   0.22912                    # 38
#XLP5+    0.64694   0.08916  -0.14925                    # 39
#XLP5-    0.70586   0.16269  -0.00910                    # 40
#XLP6+    0.81593   0.15154  -0.08581                    # 41
#XLP6-    0.60100   0.19500  -0.20814                    # 42
#XLP7+    0.53649   0.10894  -0.12517                    # 43
#XLP7-    0.51638   0.12049   0.03253                    # 44
#END
```

S19. Optimized crystal structure coordinates for azidoformamidine – dinitramic acid (cocrystal form).

```
data_N3F_DNH_1
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.15441E+01 E(coul)=-2.23188E+01 E(vdW)=-1.92253E+01 Density= 1.73309
;
_cell_length_a    6.658
_cell_length_b   13.383
_cell_length_c   10.250
_cell_angle_alpha    90.00
_cell_angle_beta     53.73
```

```
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       -0.13353   0.24797   0.09056                    #  1
N'2      -0.04395   0.18509  -0.02543                    #  2
H*3       -0.06937   0.11321   0.01459                    #  3
N4       -0.25929   0.23067   0.25396                    #  4
N'5      -0.11948   0.35297   0.06238                    #  5
N6       -0.01711   0.37651  -0.08166                    #  6
N'7       0.07197   0.40732  -0.20756                    #  7
H*8       -0.24362   0.16196   0.28764                    #  8
H*9       -0.27799   0.28829   0.32415                    #  9
#XC1      -0.15900   0.25793   0.12577                    # 10
#XN'2     -0.03421   0.19545  -0.04788                    # 11
#XH*3      -0.05963   0.11331   0.00260                    # 12
#XN4      -0.21559   0.23443   0.23258                    # 13
#XN'5     -0.13107   0.35613   0.08352                    # 14
#XN6      -0.02188   0.36917  -0.07587                    # 15
#XN'7      0.06838   0.41966  -0.19749                    # 16
#XH*8      -0.24193   0.16436   0.28907                    # 17
#XH*9      -0.28235   0.29179   0.33223                    # 18
#XLP1+     -0.09649   0.26371   0.07182                    # 19
#XLP1-     -0.16361   0.25499   0.09928                    # 20
#XLP2+     -0.05881   0.18476   0.00786                    # 21
#XLP2-     -0.03036   0.19140  -0.03601                    # 22
#XLP4+     -0.16165   0.22689   0.25367                    # 23
#XLP4-     -0.36452   0.22634   0.28243                    # 24
#XLP5+     -0.06423   0.36069   0.07772                    # 25
#XLP5-     -0.20425   0.35930   0.09707                    # 26
#XLP6+     -0.02899   0.37927  -0.07212                    # 27
#XLP6-     -0.01724   0.38149  -0.07142                    # 28
#XLP7+      0.14818   0.41921  -0.23248                    # 29
#XLP7-      0.02005   0.41834  -0.21930                    # 30
N1+       0.77241  -0.10851   0.34470                     # 31
N'2+      0.82055  -0.14876   0.45591                     # 32
O3+       0.76131  -0.09988   0.57223                     # 33
O4+       0.90766  -0.23281   0.41795                     # 34
N'5+      0.81943  -0.00276   0.30320                     # 35
O6+       0.76011   0.05659   0.40856                     # 36
O7+       0.90579   0.01213   0.16176                     # 37
```

```
H*8+      0.87897  -0.14805   0.23929                                  # 38
#XN1+      0.66570  -0.11050   0.38269                                  # 39
#XN'2+     0.78453  -0.14592   0.41747                                  # 40
#XO3+      0.82622  -0.13260   0.53927                                  # 41
#XO4+      0.91891  -0.20422   0.36681                                  # 42
#XN'5+     0.78374  -0.04253   0.30932                                  # 43
#XO6+      0.82477   0.05774   0.34018                                  # 44
#XO7+      0.91757  -0.02904   0.18358                                  # 45
#XH*8+     0.89460  -0.15096   0.22853                                   # 46
#XLP1+     0.87899  -0.04739   0.33680                                   # 47
#XLP1-     0.76800  -0.09036   0.36552                                  # 48
#XLP2+     0.89246  -0.15479   0.47893                                   # 49
#XLP2-     0.74366  -0.11919   0.42295                                  # 50
#XLP3+     0.72216  -0.07960   0.49841                                   # 51
#XLP3-     0.67777  -0.20672   0.58075                                  # 52
#XLP4+     0.88817  -0.20507   0.45050                                   # 53
#XLP4-     0.89422  -0.19019   0.32807                                  # 54
#XLP5+     0.89100   0.03653   0.27882                                   # 55
#XLP5-     0.74317  -0.05600   0.35686                                  # 56
#XLP6+     0.72166  -0.01430   0.43011                                   # 57
#XLP6-     0.67572   0.06186   0.29983                                  # 58
#XLP7+     0.88641   0.02486   0.21000                                   # 59
#XLP7-     0.89328  -0.06817   0.20044                                  # 60
#END

data_N3F_DNH_2
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.15382E+01 E(coul)=-2.31785E+01 E(vdW)=-1.83596E+01 Density= 1.68956
;
_cell_length_a    9.661
_cell_length_b    8.781
_cell_length_c    5.394
_cell_angle_alpha    97.08
_cell_angle_beta    110.01
_cell_angle_gamma   113.07
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.42644   0.20223   0.01043                                 #  1
N'2       0.54656   0.19546   0.19788                                 #  2
H*3       0.50572   0.11522   0.30683                                  #  3
```

```
N4        0.25804   0.11487  -0.06210                    #  4
N'5       0.45486   0.30632  -0.16775                    #  5
N6        0.60344   0.38583  -0.12598                    #  6
N'7       0.73323   0.46450  -0.10830                    #  7
H*8       0.22289   0.06204   0.07580                    #  8
H*9       0.18438   0.15822  -0.18079                    #  9
#XC1      0.39001   0.19694  -0.02854                    # 10
#XN'2     0.56980   0.21026   0.18705                    # 11
#XH*3     0.51808   0.12087   0.31468                    # 12
#XN4      0.27944   0.14401  -0.03224                    # 13
#XN'5     0.43293   0.30278  -0.18292                    # 14
#XN6      0.59753   0.37638  -0.11667                    # 15
#XN'7     0.72265   0.47391  -0.13344                    # 16
#XH*8     0.22133   0.06529   0.07292                    # 17
#XH*9     0.17598   0.15901  -0.19067                    # 18
#XLP1+    0.44513   0.23843   0.01306                    # 19
#XLP1-    0.41793   0.19084  -0.02759                    # 20
#XLP2+    0.51198   0.18705   0.18645                    # 21
#XLP2-    0.55730   0.20915   0.19781                    # 22
#XLP4+    0.25614   0.16997   0.02738                    # 23
#XLP4-    0.23062   0.04846  -0.14288                    # 24
#XLP5+    0.43744   0.34692  -0.13467                    # 25
#XLP5-    0.42036   0.26211  -0.25036                    # 26
#XLP6+    0.59367   0.38148  -0.14087                    # 27
#XLP6-    0.59266   0.39058  -0.13491                    # 28
#XLP7+    0.75753   0.52052  -0.06566                    # 29
#XLP7-    0.74665   0.44318  -0.17235                    # 30
N1+       0.87172   0.25807   0.54938                    # 31
N'2+      0.82014   0.11203   0.65842                    # 32
O3+       0.92139   0.06729   0.77524                    # 33
O4+       0.67622   0.05798   0.62628                    # 34
N'5+      0.98092   0.27123   0.41296                    # 35
O6+       1.09371   0.23790   0.51217                    # 36
O7+       0.94596   0.32506   0.21447                    # 37
H*8+      0.76628   0.25415   0.41054                    # 38
#XN1+     0.91471   0.31537   0.64858                    # 39
#XN'2+    0.83125   0.17736   0.63888                    # 40
#XO3+     0.85106   0.03584   0.72722                    # 41
#XO4+     0.70021   0.09817   0.55071                    # 42
#XN'5+    0.94511   0.29009   0.46505                    # 43
#XO6+     1.06068   0.24339   0.40720                    # 44
#XO7+     0.89313   0.28918   0.25618                    # 45
#XH*8+    0.75516   0.24987   0.39294                    # 46
#XLP1+    0.90775   0.18351   0.44157                    # 47
#XLP1-    0.89937   0.24624   0.56067                    # 48
#XLP2+    0.78931   0.02918   0.64448                    # 49
#XLP2-    0.88092   0.21165   0.65002                    # 50
#XLP3+    0.95022   0.16937   0.71111                    # 51
#XLP3-    0.81938   0.11442   0.90037                    # 52
#XLP4+    0.72333   0.05016   0.65147                    # 53
#XLP4-    0.72114   0.15582   0.51719                    # 54
#XLP5+    1.00000   0.23778   0.32283                    # 55
```

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#XLP5-      0.95051   0.28055   0.54378                    # 56
#XLP6+      1.02212   0.24057   0.60133                    # 57
#XLP6-      1.11515   0.40727   0.44881                    # 58
#XLP7+      0.97654   0.30087   0.26489                    # 59
#XLP7-      0.85551   0.28887   0.31204                    # 60
#END

data_N3F_DNH_3
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.14380E+01 E(coul)=-2.30428E+01 E(vdW)=-1.83952E+01 Density= 1.73057
;
_cell_length_a    9.307
_cell_length_b   15.168
_cell_length_c    5.469
_cell_angle_alpha    90.00
_cell_angle_beta     72.76
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.05338  -0.13807   0.50985                   #  1
N'2        0.17114  -0.13351   0.58457                   #  2
H*3         0.16258  -0.17268   0.73982                   #  3
N4        -0.07402  -0.18873   0.60459                   #  4
N'5        0.04104  -0.08883   0.29477                   #  5
N6         0.15360  -0.04321   0.18852                   #  6
N'7        0.24838   0.00085   0.07602                   #  7
H*8       -0.09256  -0.21416   0.78174                    #  8
H*9       -0.16616  -0.17277   0.55220                    #  9
#XC1        0.02029  -0.14276   0.50582                    # 10
#XN'2       0.18865  -0.12544   0.55020                    # 11
#XH*3        0.17216  -0.16930   0.73549                    # 12
#XN4       -0.06843  -0.17341   0.61218                    # 13
#XN'5       0.02077  -0.09173   0.30076                    # 14
#XN6        0.15166  -0.04791   0.20430                    # 15
#XN'7       0.23403   0.00457   0.06007                    # 16
#XH*8      -0.09569  -0.21270   0.78010                    # 17
#XH*9      -0.17477  -0.17290   0.55022                    # 18
#XLP1+      0.05422  -0.11979   0.49198                    # 19
```

```
#XLP1-      0.05271  -0.14436   0.48037                    # 20
#XLP2+      0.13987  -0.13931   0.60685                    # 21
#XLP2-      0.17539  -0.12644   0.57320                    # 22
#XLP4+     -0.11006  -0.16137   0.69310                    # 23
#XLP4-     -0.06353  -0.22280   0.55389                    # 24
#XLP5+     -0.00026  -0.06980   0.34214                    # 25
#XLP5-      0.03278  -0.11260   0.24746                    # 26
#XLP6+      0.14653  -0.04593   0.18315                    # 27
#XLP6-      0.14040  -0.04154   0.18951                    # 28
#XLP7+      0.24239   0.02935   0.09185                    # 29
#XLP7-      0.27754  -0.00948  -0.00022                    # 30
N1+       -0.52403   0.87724   0.27284                    # 31
N'2+      -0.42783   0.87670   0.44012                    # 32
O3+       -0.29895   0.85367   0.35315                    # 33
O4+       -0.49259   0.90518   0.65267                    # 34
N'5+      -0.51275   0.80419   0.09499                    # 35
O6+       -0.38997   0.77596  -0.01675                    # 36
O7+       -0.63506   0.78353   0.07365                    # 37
H*8+      -0.63296   0.87983   0.38700                    # 38
#XN1+     -0.49942   0.90595   0.20491                    # 39
#XN'2+    -0.46810   0.88917   0.38681                    # 40
#XO3+     -0.33856   0.85744   0.45338                    # 41
#XO4+     -0.52873   0.88965   0.58480                    # 42
#XN'5+    -0.52824   0.83782   0.14239                    # 43
#XO6+     -0.44927   0.76291   0.00341                    # 44
#XO7+     -0.63062   0.80265   0.17068                    # 45
#XH*8+    -0.64306   0.87803   0.40052                    # 46
#XLP1+    -0.49312   0.81032   0.24397                    # 47
#XLP1-    -0.49614   0.86568   0.24485                    # 48
#XLP2+    -0.40014   0.85713   0.52228                    # 49
#XLP2-    -0.45538   0.88457   0.30512                    # 50
#XLP3+    -0.36645   0.85998   0.24811                    # 51
#XLP3-    -0.34695   0.94116   0.48714                    # 52
#XLP4+    -0.45063   0.89117   0.59957                    # 53
#XLP4-    -0.56311   0.89215   0.51987                    # 54
#XLP5+    -0.51142   0.76211   0.07002                    # 55
#XLP5-    -0.49213   0.85319   0.15574                    # 56
#XLP6+    -0.40442   0.82755   0.09377                    # 57
#XLP6-    -0.50317   0.80778  -0.14776                    # 58
#XLP7+    -0.58437   0.77698   0.05603                    # 59
#XLP7-    -0.63408   0.83155   0.23143                    # 60
#END

data_N3F_DNH_4
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.14356E+01 E(coul)=-2.27358E+01 E(vdW)=-1.86998E+01 Density= 1.70560
;
_cell_length_a   17.940
_cell_length_b    5.369
_cell_length_c   16.923
```

```
_cell_angle_alpha    90.00
_cell_angle_beta    113.35
_cell_angle_gamma    90.00
_cell_formula_units_Z  8
_symmetry_space_group_name_H-M 'C 2/C   '
_symmetry_Int_Tables_number  15
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,y,1/2-z
  3 -x,-y,-z
  4 x,-y,1/2+z
  5 1/2+x,1/2+y,z
  6 1/2-x,1/2+y,1/2-z
  7 1/2-x,1/2-y,-z
  8 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.21124   0.75111   0.60383                    #  1
N'2       0.26962   0.63048   0.59631                    #  2
H*3       0.24903   0.48595   0.55406                    #  3
N4        0.12869   0.71490   0.56201                    #  4
N'5       0.22603   0.96157   0.65944                    #  5
N6        0.29914   1.01616   0.69795                    #  6
N'7       0.36308   1.08410   0.73658                    #  7
H*8       0.10995   0.54867   0.53312                    #  8
H*9       0.09207   0.79850   0.58656                    #  9
#XC1      0.19342   0.76866   0.60208                    # 10
#XN'2     0.28127   0.65679   0.60383                    # 11
#XH*3     0.25506   0.48596   0.55670                    # 12
#XN4      0.13847   0.70149   0.57612                    # 13
#XN'5     0.21519   0.96377   0.65807                    # 14
#XN6      0.29620   1.00205   0.69304                    # 15
#XN'7     0.35787   1.10470   0.74186                    # 16
#XH*8     0.10912   0.55116   0.53483                    # 17
#XH*9     0.08794   0.80374   0.58719                    # 18
#XLP1+    0.21989   0.76452   0.62200                    # 19
#XLP1-    0.20773   0.78269   0.59876                    # 20
#XLP2+    0.25241   0.62100   0.59249                    # 21
#XLP2-    0.27478   0.63871   0.60317                    # 22
#XLP4+    0.12517   0.63230   0.58843                    # 23
#XLP4-    0.11742   0.77040   0.52993                    # 24
#XLP5+    0.21579   0.92453   0.67958                    # 25
#XLP5-    0.21070   1.01818   0.63870                    # 26
#XLP6+    0.29449   1.02489   0.69607                    # 27
#XLP6-    0.29369   1.01969   0.70059                    # 28
#XLP7+    0.37355   1.06353   0.76407                    # 29
#XLP7-    0.37132   1.15280   0.72677                    # 30
N1+       0.57124   0.45936  -0.12649                    # 31
```

```
N'2+      0.59331   0.28462  -0.05490                                  # 32
O3+       0.54061   0.20508  -0.03472                                  # 33
O4+       0.66522   0.23118  -0.02659                                  # 34
N'5+      0.51206   0.65339  -0.13370                                  # 35
O6+       0.45353   0.60030  -0.11918                                  # 36
O7+       0.52891   0.84986  -0.15880                                  # 37
H*8+      0.62332   0.54553  -0.12273                                   # 38
#XN1+      0.55358   0.39685  -0.15542                                    # 39
#XN'2+     0.59028   0.32760  -0.08689                                    # 40
#XO3+      0.57485   0.20997  -0.01830                                    # 41
#XO4+      0.65310   0.32974  -0.04623                                    # 42
#XN'5+     0.53274   0.58876  -0.14270                                    # 43
#XO6+      0.46892   0.69075  -0.12104                                    # 44
#XO7+      0.55562   0.77222  -0.14078                                    # 45
#XH*8+      0.62856   0.55652  -0.12043                                     # 46
#XLP1+      0.54661   0.56462  -0.09004                                     # 47
#XLP1-     0.55645   0.45839  -0.12109                                    # 48
#XLP2+      0.60511   0.26067  -0.01396                                     # 49
#XLP2-     0.56622   0.35029  -0.10430                                    # 50
#XLP3+      0.52921   0.31156  -0.08472                                     # 51
#XLP3-     0.59873   0.04247  -0.05702                                    # 52
#XLP4+      0.64074   0.22697  -0.02344                                     # 53
#XLP4-     0.64429   0.38945  -0.07454                                    # 54
#XLP5+      0.49864   0.74389  -0.11722                                     # 55
#XLP5-     0.53106   0.50990  -0.13841                                    # 56
#XLP6+      0.49287   0.47648  -0.11997                                     # 57
#XLP6-     0.44927   0.72085  -0.20199                                    # 58
#XLP7+      0.51278   0.80773  -0.14755                                     # 59
#XLP7-     0.57639   0.69765  -0.14040                                    # 60
#END

data_N3F_DNH_5
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.14079E+01 E(coul)=-2.29645E+01 E(vdW)=-1.84434E+01 Density= 1.69807
;
_cell_length_a    9.330
_cell_length_b    8.423
_cell_length_c    5.446
_cell_angle_alpha    88.02
_cell_angle_beta    102.45
_cell_angle_gamma   115.70
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,-y,-z
loop_
_atom_site_label
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.58071   0.29502   0.56176                 #  1
N'2       0.46145   0.30447   0.62977                 #  2
H*3       0.50002   0.38750   0.78677                 #  3
N4        0.74562   0.38286   0.66555                 #  4
N'5       0.55502   0.18680   0.34580                 #  5
N6        0.40960   0.10659   0.23197                 #  6
N'7       0.28278   0.02690   0.11290                 #  7
H*8       0.77919   0.43809   0.84254                 #  8
H*9       0.81967   0.33683   0.61575                 #  9
#XC1      0.61672   0.29984   0.55965                 # 10
#XN'2     0.43875   0.28933   0.59451                 # 11
#XH*3     0.48790   0.38187   0.78175                 # 12
#XN4      0.72508   0.35339   0.67078                 # 13
#XN'5     0.57669   0.19014   0.35278                 # 14
#XN6      0.41523   0.11633   0.24806                 # 15
#XN'7     0.29349   0.01695   0.09737                 # 16
#XH*8     0.78082   0.43472   0.84086                 # 17
#XH*9     0.82802   0.33588   0.61416                 # 18
#XLP1+    0.56304   0.25803   0.54192                 # 19
#XLP1-    0.58890   0.30629   0.53379                 # 20
#XLP2+    0.49552   0.31276   0.65344                 # 21
#XLP2-    0.45112   0.29050   0.61760                 # 22
#XLP4+    0.74877   0.32717   0.74983                 # 23
#XLP4-    0.77126   0.45004   0.62000                 # 24
#XLP5+    0.57324   0.14535   0.39117                 # 25
#XLP5-    0.58821   0.23114   0.30295                 # 26
#XLP6+    0.41918   0.11086   0.22734                 # 27
#XLP6-    0.42040   0.10157   0.23322                 # 28
#XLP7+    0.25999  -0.03000   0.12492                 # 29
#XLP7-    0.26899   0.04826   0.03866                 # 30
N1+       0.13936   0.24057   0.64575                 # 31
N'2+      0.18371   0.38690   0.82637                 # 32
O3+       0.08022   0.43064   0.84960                 # 33
O4+       0.32488   0.44202   0.94374                 # 34
N'5+      0.03215   0.22908   0.40201                 # 35
O6+      -0.08221   0.26150   0.39480                 # 36
O7+       0.07061   0.17723   0.23178                 # 37
H*8+      0.24510   0.24637   0.61231                 # 38
#XN1+     0.09833   0.18127   0.69295                 # 39
#XN'2+    0.17558   0.32106   0.78619                 # 40
#XO3+     0.14921   0.46310   0.87578                 # 41
#XO4+     0.30323   0.40235   0.83940                 # 42
#XN'5+    0.06825   0.20929   0.48566                 # 43
#XO6+    -0.04838   0.25733   0.32252                 # 44
#XO7+     0.12138   0.21298   0.33022                 # 45
#XH*8+    0.25610   0.25093   0.60645                 # 46
#XLP1+    0.10105   0.31745   0.51534                 # 47
#XLP1-    0.11125   0.25239   0.63166                 # 48
#XLP2+    0.21095   0.47093   0.85545                 # 49
```

```
#XLP2-      0.12753   0.28621   0.74333                    # 50
#XLP3+      0.05633   0.32819   0.74236                    # 51
#XLP3-      0.18292   0.38128   1.06591                    # 52
#XLP4+      0.27748   0.44960   0.92372                    # 53
#XLP4-      0.28510   0.34445   0.77697                    # 54
#XLP5+      0.01236   0.26412   0.29937                    # 55
#XLP5-      0.06193   0.21790   0.55966                    # 56
#XLP6+     -0.01145   0.25761   0.55258                    # 57
#XLP6-     -0.09589   0.09094   0.28524                    # 58
#XLP7+      0.03880   0.20104   0.25541                    # 59
#XLP7-      0.15843   0.21255   0.42230                    # 60
#END
```

S20. Optimized crystal structure coordinates for guanidine – dinitramic acid (cocrystal form).

```
data_G_DNH_1
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-5.21122E+01 E(coul)=-3.12002E+01 E(vdW)=-2.09119E+01 Density= 1.82449
;
_cell_length_a    6.463
_cell_length_b    9.113
_cell_length_c   10.790
_cell_angle_alpha    90.00
_cell_angle_beta    107.90
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.45358  -0.14263   0.73538                   #  1
N'2       0.53598  -0.24337   0.81932                   #  2
H*3       0.62495  -0.19958   0.90643                    #  3
N4        0.34649  -0.17931   0.60608                   #  4
H*5       0.21019  -0.12035   0.56339                    #  5
H*6       0.32364  -0.28899   0.59372                    #  6
N7        0.45487   0.00871   0.75732                   #  7
H*8       0.55497   0.04091   0.84499                    #  8
H*9       0.46847   0.07207   0.68298                    #  9
#XC1       0.42563  -0.13414   0.71009                     # 10
#XN'2      0.52677  -0.25666   0.81137                     # 11
```

```
#XH*3      0.62421  -0.21682   0.90668                    # 12
#XN4       0.32902  -0.17383   0.60871                    # 13
#XH*5      0.20405  -0.12608   0.56120                    # 14
#XH*6      0.32456  -0.27968   0.59669                    # 15
#XN7       0.46248   0.00134   0.75010                    # 16
#XH*8      0.55339   0.04122   0.84441                    # 17
#XH*9      0.46884   0.07279   0.68900                    # 18
#XLP1+     0.42534  -0.14241   0.74220                    # 19
#XLP1-     0.47726  -0.14991   0.72180                    # 20
#XLP2+     0.50901  -0.25827   0.81420                    # 21
#XLP2-     0.55762  -0.24159   0.81259                    # 22
#XLP4+     0.24995  -0.19112   0.61306                    # 23
#XLP4-     0.39908  -0.16664   0.57639                    # 24
#XLP7+     0.38329   0.02465   0.75517                    # 25
#XLP7-     0.53938   0.01339   0.75082                    # 26
N1+       -0.01959   0.04632   0.80107                    # 27
N'2+       0.15774   0.10792   0.90667                    # 28
O3+        0.20177   0.23571   0.90198                    # 29
O4+        0.23397   0.01856   0.99268                    # 30
N'5+      -0.03976   0.08925   0.66774                    # 31
O6+       -0.00990   0.21570   0.64592                    # 32
O7+       -0.09737  -0.01276   0.59184                    # 33
H*8+      -0.00398  -0.06526   0.80633                    # 34
#XN1+     -0.09432   0.07384   0.80917                    # 35
#XN'2+     0.07853   0.07840   0.88026                    # 36
#XO3+      0.24590   0.18675   0.93024                    # 37
#XO4+      0.18562  -0.00203   0.93682                    # 38
#XN'5+     -0.06133   0.06518   0.71105                    # 39
#XO6+      -0.01159   0.16242   0.61875                    # 40
#XO7+      -0.05136  -0.02442   0.65014                    # 41
#XH*8+      0.00242  -0.07578   0.80617                    # 42
#XLP1+      0.07064   0.08534   0.74145                    # 43
#XLP1-     -0.00753   0.07601   0.79043                    # 44
#XLP2+      0.26036   0.12328   0.93338                    # 45
#XLP2-      0.03333   0.10130   0.84807                    # 46
#XLP3+      0.07801   0.19010   0.83823                    # 47
#XLP3-      0.14887   0.16484   1.01592                    # 48
#XLP4+      0.23947   0.06433   0.97525                    # 49
#XLP4-      0.11533  -0.02361   0.89907                    # 50
#XLP5+      0.00156   0.09883   0.62030                    # 51
#XLP5-     -0.05215   0.09322   0.74467                    # 52
#XLP6+     -0.01032   0.18176   0.73138                    # 53
#XLP6-     -0.21445   0.13051   0.57640                    # 54
#XLP7+     -0.07156   0.03494   0.59898                    # 55
#XLP7-     -0.04973  -0.03921   0.69939                    # 56
#END

data_G_DNH_2
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-5.20866E+01 E(coul)=-3.06090E+01 E(vdW)=-2.14776E+01 Density= 1.83943
```

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_cell_length_a    9.089
_cell_length_b    6.726
_cell_length_c    6.535
_cell_angle_alpha    69.06
_cell_angle_beta    112.77
_cell_angle_gamma    73.53
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P -1    '
_symmetry_Int_Tables_number   2
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,-y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.59337   0.19638   0.33132                    #  1
N'2       0.42091   0.26929   0.21057                    #  2
H*3       0.36774   0.31618   0.02077                     #  3
N4        0.68806   0.14970   0.58412                    #  4
H*5       0.81444   0.00056   0.70677                     #  5
H*6       0.61052   0.15398   0.66136                     #  6
N7        0.70726   0.15248   0.23920                    #  7
H*8       0.63999   0.21465   0.04595                     #  8
H*9       0.80845   0.19485   0.29784                     #  9
#XC1      0.62768   0.17560   0.37899                      # 10
#XN'2     0.41818   0.26579   0.23252                      # 11
#XH*3      0.35306   0.31899   0.02819                      # 12
#XN4      0.69687   0.12664   0.59042                      # 13
#XH*5      0.81315  -0.00416   0.71615                      # 14
#XH*6      0.61611   0.15138   0.65306                      # 15
#XN7      0.70337   0.16693   0.24626                     # 16
#XH*8      0.64119   0.21305   0.04764                      # 17
#XH*9      0.80476   0.19184   0.28962                      # 18
#XLP1+     0.59842   0.15961   0.34186                       # 19
#XLP1-     0.58852   0.23307   0.33545                      # 20
#XLP2+     0.42087   0.24384   0.24173                       # 21
#XLP2-     0.41975   0.29786   0.20359                      # 22
#XLP4+     0.70590   0.03565   0.64614                       # 23
#XLP4-     0.70165   0.22455   0.58062                      # 24
#XLP7+     0.74670   0.06644   0.28415                       # 25
#XLP7-     0.68706   0.25379   0.18777                      # 26
N1+       0.17875   0.44281   0.34365                     # 27
N'2+      0.26853   0.40490   0.60411                     # 28
O3+       0.17787   0.51526   0.66041                     # 29
O4+       0.42963   0.24975   0.74014                     # 30
N'5+      0.04264   0.69013   0.12103                     # 31
O6+      -0.06423   0.82095   0.14269                      # 32
O7+       0.05065   0.72827  -0.07030                      # 33
```

```
H*8+      0.27866   0.37873   0.31163                                  # 34
#XN1+      0.13460   0.39699   0.34832                                  # 35
#XN'2+     0.24467   0.38405   0.52346                                  # 36
#XO3+      0.25371   0.46505   0.70242                                  # 37
#XO4+      0.38916   0.30565   0.61995                                  # 38
#XN'5+     0.08469   0.58604   0.18136                                  # 39
#XO6+     -0.04079   0.83692   0.07262                                  # 40
#XO7+      0.11811   0.64789   0.04032                                  # 41
#XH*8+     0.28943   0.37697   0.30883                                  # 42
#XLP1+     0.13840   0.62796   0.27991                                  # 43
#XLP1-     0.15163   0.48646   0.34045                                  # 44
#XLP2+     0.31270   0.43189   0.68601                                  # 45
#XLP2-     0.18678   0.42539   0.46360                                  # 46
#XLP3+     0.12433   0.52266   0.49507                                  # 47
#XLP3-     0.29604   0.23952   0.81712                                  # 48
#XLP4+     0.38227   0.31056   0.72973                                  # 49
#XLP4-     0.35416   0.31507   0.52510                                  # 50
#XLP5+     0.01670   0.80564   0.05301                                  # 51
#XLP5-     0.08901   0.54884   0.25453                                  # 52
#XLP6+     0.02331   0.65022   0.27903                                  # 53
#XLP6-    -0.11951   0.76423  -0.07154                                  # 54
#XLP7+     0.02652   0.75975  -0.03104                                  # 55
#XLP7-     0.16537   0.55345   0.12137                                  # 56
#END

data_G_DNH_3
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-5.20782E+01 E(coul)=-3.10375E+01 E(vdW)=-2.10407E+01 Density= 1.82759
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_cell_length_a    6.453
_cell_length_b    9.134
_cell_length_c   10.730
_cell_angle_alpha    90.00
_cell_angle_beta    107.30
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.77569   0.14089   0.73395                                  #  1
```

```
N'2       0.77844   0.24144   0.81815                # 2
H*3       0.78178   0.19776   0.90626                # 3
N4        0.74666   0.17717   0.60365                # 4
H*5       0.83933   0.11947   0.55956                # 5
H*6       0.75361   0.28671   0.59053                # 6
N7        0.80123  -0.00983   0.75649                # 7
H*8       0.79378  -0.04206   0.84525                # 8
H*9       0.71203  -0.07411   0.68300                # 9
#XC1      0.77739   0.13244   0.70844                # 10
#XN'2     0.77897   0.25471   0.81005                # 11
#XH*3     0.78231   0.21497   0.90641                # 12
#XN4      0.76691   0.17195   0.60604                # 13
#XH*5     0.84300   0.12523   0.55726                # 14
#XH*6     0.75603   0.27745   0.59354                # 15
#XN7      0.78597  -0.00265   0.74938                # 16
#XH*8     0.79476  -0.04236   0.84465                # 17
#XH*9     0.71796  -0.07477   0.68901                # 18
#XLP1+    0.81088   0.14110   0.74034                # 19
#XLP1-    0.73783   0.14770   0.72074                # 20
#XLP2+    0.79954   0.25656   0.81261                # 21
#XLP2-    0.74997   0.23932   0.81176                # 22
#XLP4+    0.84961   0.19020   0.60920                # 23
#XLP4-    0.66380   0.16353   0.57490                # 24
#XLP7+    0.87061  -0.02489   0.75343                # 25
#XLP7-    0.71056  -0.01559   0.75122                # 26
N1+       0.67927   0.04370   0.19843                # 27
N'2+      0.79021   0.08766   0.33227                # 28
O3+       0.83968   0.21424   0.35391                # 29
O4+       0.80913  -0.01382   0.40865                # 30
N'5+      0.75207   0.10548   0.09338                # 31
O6+       0.79880   0.23334   0.09788                # 32
O7+       0.74514   0.01608   0.00787                # 33
H*8+      0.69168  -0.06755   0.19378                # 34
#XN1+     0.59563   0.07053   0.18949                # 35
#XN'2+    0.72606   0.06306   0.28859                # 36
#XO3+     0.86579   0.16133   0.38149                # 37
#XO4+     0.79792  -0.02567   0.35042                # 38
#XN'5+    0.69905   0.07568   0.11942                # 39
#XO6+     0.81606   0.18456   0.07005                # 40
#XO7+     0.75215  -0.00429   0.06378                # 41
#XH*8+    0.69845  -0.07799   0.19405                # 42
#XLP1+    0.81546   0.08990   0.17818                # 43
#XLP1-    0.69940   0.07447   0.19639                # 44
#XLP2+    0.87856   0.09797   0.38034                # 45
#XLP2-    0.70155   0.09079   0.25471                # 46
#XLP3+    0.75526   0.17956   0.26804                # 47
#XLP3-    0.70422   0.12838   0.42252                # 48
#XLP4+    0.82722   0.03389   0.40147                # 49
#XLP4-    0.75106  -0.04088   0.30092                # 50
#XLP5+    0.82858   0.12132   0.06731                # 51
#XLP5-    0.68504   0.09850   0.15131                # 52
#XLP6+    0.73821   0.18753   0.16120                # 53
```

```
#XLP6-      0.63405   0.16116  -0.01694                    # 54
#XLP7+      0.76715   0.06195   0.02525                    # 55
#XLP7-      0.71918  -0.02599   0.10127                    # 56
#END

data_G_DNH_4
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-5.17455E+01 E(coul)=-3.21921E+01 E(vdW)=-1.95534E+01 Density= 1.76977
;
_cell_length_a    7.289
_cell_length_b   12.653
_cell_length_c   13.670
_cell_angle_alpha    90.00
_cell_angle_beta     81.57
_cell_angle_gamma    90.00
_cell_formula_units_Z  8
_symmetry_space_group_name_H-M 'C 2/C   '
_symmetry_Int_Tables_number  15
loop_
_symmetry_equiv_pos_as_xyz
  1 x,y,z
  2 -x,y,1/2-z
  3 -x,-y,-z
  4 x,-y,1/2+z
  5 1/2+x,1/2+y,z
  6 1/2-x,1/2+y,1/2-z
  7 1/2-x,1/2-y,-z
  8 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.47429   0.76953   0.53374                   #  1
N'2       0.46523   0.78371   0.44152                   #  2
H*3       0.53547   0.72616   0.39911                    #  3
N4        0.40501   0.84578   0.60308                   #  4
H*5       0.33684   0.81680   0.66745                    #  5
H*6       0.33314   0.90286   0.57313                    #  6
N7        0.54749   0.68205   0.57728                   #  7
H*8       0.62061   0.63198   0.52865                    #  8
H*9       0.61254   0.69868   0.63612                    #  9
#XC1       0.46316   0.77541   0.55408                    # 10
#XN'2      0.45312   0.79332   0.44218                    # 11
#XH*3       0.52587   0.73435   0.39285                    # 12
#XN4       0.39289   0.83816   0.60644                    # 13
#XH*5       0.32950   0.81978   0.66745                    # 14
#XH*6       0.33787   0.89666   0.57485                    # 15
#XN7       0.55191   0.69151   0.57710                    # 16
#XH*8       0.61965   0.63188   0.52931                    # 17
```

```
#XH*9      0.61150   0.69473   0.63325                    # 18
#XLP1+     0.44949   0.75990   0.53473                    # 19
#XLP1-     0.49365   0.78587   0.53435                    # 20
#XLP2+     0.43703   0.78901   0.44291                    # 21
#XLP2-     0.48567   0.79105   0.44224                    # 22
#XLP4+     0.31838   0.82896   0.61023                    # 23
#XLP4-     0.46282   0.86761   0.61467                    # 24
#XLP7+     0.49812   0.66189   0.59528                    # 25
#XLP7-     0.62050   0.69979   0.56916                    # 26
N1+       0.66977  -0.05740   0.16326                    # 27
N'2+      0.75385  -0.09423   0.24746                    # 28
O3+       0.82299  -0.03024   0.29604                    # 29
O4+       0.73351  -0.18907   0.26056                    # 30
N'5+      0.76465   0.02442   0.09991                    # 31
O6+       0.83456   0.09693   0.13790                    # 32
O7+       0.75162   0.01000   0.01302                    # 33
H*8+      0.65489  -0.12153   0.11968                    # 34
#XN1+      0.60536  -0.03536   0.18225                    # 35
#XN'2+     0.69984  -0.08757   0.22176                    # 36
#XO3+      0.82844  -0.07461   0.29155                    # 37
#XO4+      0.73064  -0.16969   0.21941                    # 38
#XN'5+     0.70749  -0.00354   0.11727                    # 39
#XO6+      0.84251   0.08008   0.09919                    # 40
#XO7+      0.74360  -0.02732   0.04237                    # 41
#XH*8+     0.65822  -0.12800   0.11500                    # 42
#XLP1+     0.80167  -0.02446   0.13970                    # 43
#XLP1-     0.69477  -0.03878   0.16862                    # 44
#XLP2+     0.82464  -0.11195   0.26666                    # 45
#XLP2-     0.69085  -0.05532   0.21307                    # 46
#XLP3+     0.75607  -0.01011   0.24229                    # 47
#XLP3-     0.67430  -0.10838   0.33845                    # 48
#XLP4+     0.76162  -0.15806   0.26865                    # 49
#XLP4-     0.69476  -0.15530   0.18974                    # 50
#XLP5+     0.83879   0.04353   0.07331                    # 51
#XLP5-     0.69553  -0.00397   0.14921                    # 52
#XLP6+     0.76090   0.04296   0.17631                    # 53
#XLP6-     0.69417   0.10990   0.06701                    # 54
#XLP7+     0.77862   0.02881   0.03628                    # 55
#XLP7-     0.70379  -0.05613   0.06642                    # 56
#END

data_G_DNH_5
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-5.17218E+01 E(coul)=-3.19394E+01 E(vdW)=-1.97824E+01 Density= 1.83337
;
_cell_length_a    7.124
_cell_length_b    6.852
_cell_length_c    8.038
_cell_angle_alpha    90.00
_cell_angle_beta     50.08
```

```
_cell_angle_gamma    90.00
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P 21    '
_symmetry_Int_Tables_number   4
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1       -0.31573   0.72316   0.01938                    #  1
N'2      -0.28795   0.90601   0.03341                    #  2
H*3       -0.10741   0.94410  -0.06905                     #  3
N4       -0.54633   0.63731   0.16303                    #  4
H*5       -0.58527   0.53781   0.09569                     #  5
H*6       -0.68046   0.73780   0.25472                     #  6
N7       -0.13521   0.58965  -0.13105                    #  7
H*8        0.03808   0.63997  -0.21860                     #  8
H*9       -0.15612   0.45288  -0.07320                     #  9
#XC1      -0.34736   0.69046   0.03090                      # 10
#XN'2     -0.31423   0.91205   0.04959                      # 11
#XH*3      -0.12486   0.96196  -0.05597                       # 12
#XN4      -0.54364   0.63450   0.14508                      # 13
#XH*5      -0.59586   0.54163   0.09975                       # 14
#XH*6      -0.66711   0.73114   0.24375                       # 15
#XN7       -0.14879   0.59010  -0.11099                      # 16
#XH*8       0.03714   0.63912  -0.21896                       # 17
#XH*9      -0.14797   0.45796  -0.08175                       # 18
#XLP1+     -0.31703   0.72994  -0.00620                        # 19
#XLP1-     -0.33135   0.71714   0.05720                       # 20
#XLP2+     -0.31858   0.91669   0.03688                        # 21
#XLP2-     -0.28680   0.89737   0.05350                       # 22
#XLP4+     -0.58326   0.65754   0.10779                        # 23
#XLP4-     -0.55119   0.59490   0.22325                       # 24
#XLP7+     -0.14640   0.57234  -0.18188                        # 25
#XLP7-     -0.10910   0.57736  -0.07763                       # 26
N1+       0.37531   0.18041   0.34734                     # 27
N'2+      0.16415   0.08187   0.53970                     # 28
O3+       0.02739   0.17433   0.70447                     # 29
O4+       0.14796  -0.08694   0.50230                      # 30
N'5+      0.51202   0.31758   0.37241                     # 31
O6+       0.40021   0.42695   0.52518                     # 32
O7+       0.73156   0.30851   0.22163                     # 33
H*8+       0.49492   0.07503   0.24089                      # 34
#XN1+      0.33030   0.23120   0.32505                       # 35
#XN'2+     0.23179   0.10989   0.45263                       # 36
#XO3+      0.04491   0.09379   0.68475                       # 37
#XO4+      0.24760  -0.04466   0.44460                       # 38
#XN'5+     0.47814   0.27682   0.33416                       # 39
```

```
#XO6+      0.49843   0.40109   0.46664                    # 40
#XO7+      0.66499   0.23817   0.24387                    # 41
#XH*8+     0.50727   0.06338   0.23423                    # 42
#XLP1+     0.41733   0.21482   0.44803                    # 43
#XLP1-     0.35692   0.20766   0.38645                    # 44
#XLP2+     0.11293   0.03129   0.62805                    # 45
#XLP2-     0.24922   0.17146   0.44401                    # 46
#XLP3+     0.16385   0.23403   0.56794                    # 47
#XLP3-    -0.05308   0.05899   0.59859                    # 48
#XLP4+     0.12060  -0.03844   0.55349                    # 49
#XLP4-     0.32235  -0.00602   0.37153                    # 50
#XLP5+     0.56876   0.34016   0.40884                    # 51
#XLP5-     0.39977   0.27348   0.37160                    # 52
#XLP6+     0.31942   0.33945   0.49312                    # 53
#XLP6-     0.58685   0.49260   0.29084                    # 54
#XLP7+     0.66844   0.33277   0.29003                    # 55
#XLP7-     0.61308   0.19098   0.23171                    # 56
#END
```

S21. Optimized crystal structure coordinates for nitroformamidine – dinitramic acid (cocrystal form).

```
data_NO2F_DNH_1
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.64049E+01 E(coul)=-2.41826E+01 E(vdW)=-2.22223E+01 Density= 1.94510
;
_cell_length_a    8.128
_cell_length_b   15.825
_cell_length_c    5.207
_cell_angle_alpha    90.00
_cell_angle_beta     89.53
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.20006   0.53827   0.05184                  #  1
N'2        0.28412   0.54684  -0.15135                  #  2
N3         0.09375   0.59384   0.15921                  #  3
H*4        0.07641   0.64982   0.07102                   #  4
```

```
H*5       0.03373   0.57919   0.32350                  #  5
N6        0.20995   0.45593   0.21573                  #  6
O7        0.12474   0.45209   0.41078                  #  7
O8        0.30245   0.40099   0.13714                  #  8
H*9       0.35434   0.49463  -0.18732                  #  9
#XC1      0.17455   0.57207   0.03149                  # 10
#XN'2     0.27533   0.56053  -0.16296                  # 11
#XN3      0.08014   0.59560   0.18501                  # 12
#XH*4     0.06761   0.65707   0.07393                  # 13
#XH*5     0.03552   0.59268   0.28919                  # 14
#XN6      0.20875   0.43925   0.25593                  # 15
#XO7      0.16392   0.43962   0.35315                  # 16
#XO8      0.26677   0.41186   0.19071                  # 17
#XH*9     0.36703   0.49974  -0.22661                  # 18
N1+       0.39842   0.68799  -0.42398                  # 19
N'2+      0.44775   0.74795  -0.22658                  # 20
O3+       0.54973   0.80038  -0.27988                  # 21
O4+       0.36901   0.73880  -0.02824                  # 22
N'5+      0.52492   0.65213  -0.59143                  # 23
O6+       0.63244   0.69769  -0.67090                  # 24
O7+       0.49847   0.57805  -0.64035                  # 25
H*8+      0.34046   0.63885  -0.33368                  # 26
#XN1+     0.36258   0.70915  -0.49351                  # 27
#XN'2+    0.40679   0.72907  -0.29423                  # 28
#XO3+     0.52418   0.78719  -0.18680                  # 29
#XO4+     0.37664   0.70925  -0.10464                  # 30
#XN'5+    0.46144   0.66122  -0.55261                  # 31
#XO6+     0.62479   0.66227  -0.66247                  # 32
#XO7+     0.46923   0.59428  -0.54241                  # 33
#XH*8+    0.33848   0.63359  -0.32189                  # 34
#XLP1+    0.52504   0.67381  -0.43347                  # 35
#XLP1-    0.43139   0.69598  -0.44376                  # 36
#XLP2+    0.49439   0.75890  -0.13090                  # 37
#XLP2-    0.42043   0.72894  -0.37471                  # 38
#XLP3+    0.50531   0.76157  -0.40672                  # 39
#XLP3-    0.38079   0.82062  -0.16976                  # 40
#XLP4+    0.41295   0.75162  -0.07002                  # 41
#XLP4-    0.35516   0.68850  -0.18094                  # 42
#XLP5+    0.59551   0.63335  -0.60899                  # 43
#XLP5-    0.45383   0.68747  -0.53262                  # 44
#XLP6+    0.53982   0.71872  -0.56989                  # 45
#XLP6-    0.52275   0.64436  -0.84094                  # 46
#XLP7+    0.53449   0.60073  -0.64461                  # 47
#XLP7-    0.41965   0.60842  -0.48586                  # 48
#END

data_NO2F_DNH_2
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.60276E+01 E(coul)=-2.47186E+01 E(vdW)=-2.13090E+01 Density= 1.91836
;
```

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_cell_length_a   15.125
_cell_length_b    8.782
_cell_length_c    5.267
_cell_angle_alpha    90.00
_cell_angle_beta     76.05
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 21/A  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2-x,1/2+y,-z
  3 -x,-y,-z
  4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.54454   0.28642   0.01875                        #  1
N'2       0.54805   0.20440  -0.18018                        #  2
N3        0.60961   0.37940   0.06779                        #  3
H*4       0.66931   0.38696  -0.06730                        #  4
H*5       0.59817   0.43933   0.23584                        #  5
N6        0.45773   0.29026   0.24957                        #  6
O7        0.45925   0.37262   0.43643                        #  7
O8        0.39423   0.21042   0.22697                        #  8
H*9       0.48885   0.14550  -0.16528                        #  9
#XC1      0.58157   0.30542  -0.03191                        # 10
#XN'2     0.56294   0.21061  -0.20387                        # 11
#XN3      0.61233   0.39216   0.09039                        # 12
#XH*4     0.67747   0.39423  -0.07134                        # 13
#XH*5     0.61218   0.43544   0.19102                        # 14
#XN6      0.44036   0.29411   0.30290                        # 15
#XO7      0.44366   0.33705   0.39391                        # 16
#XO8      0.40792   0.24289   0.26717                        # 17
#XH*9     0.49337   0.13249  -0.20697                        # 18
N1+       0.30511  -0.08761   0.56846                        # 19
N'2+      0.34847   0.01943   0.71201                        # 20
O3+       0.30319   0.12029   0.83283                        # 21
O4+       0.42761  -0.01416   0.69948                        # 22
N'5+      0.24114  -0.02891   0.42510                        # 23
O6+       0.18816   0.06849   0.52534                        # 24
O7+       0.24754  -0.09526   0.21814                        # 25
H*8+      0.35573  -0.14271   0.43707                        # 26
#XN1+     0.28156  -0.12109   0.65157                        # 27
#XN'2+    0.33652  -0.03682   0.67732                        # 28
#XO3+     0.34103   0.11000   0.79585                        # 29
#XO4+     0.40875  -0.03595   0.61439                        # 30
#XN'5+    0.26051  -0.07106   0.47414                        # 31
#XO6+     0.20109   0.04698   0.42180                        # 32
```

```
#XO7+      0.27997  -0.09395   0.27014                    # 33
#XH*8+     0.36127  -0.14463   0.42117                    # 34
#XLP1+     0.28803   0.01110   0.47688                    # 35
#XLP1-     0.29192  -0.05968   0.58097                    # 36
#XLP2+     0.37097   0.08205   0.71848                    # 37
#XLP2-     0.30793  -0.04049   0.67815                    # 38
#XLP3+     0.27716   0.04062   0.74480                    # 39
#XLP3-     0.35801   0.00756   0.95100                    # 40
#XLP4+     0.40435   0.02118   0.72387                    # 41
#XLP4-     0.39170  -0.07822   0.56713                    # 42
#XLP5+     0.23033   0.01871   0.34253                    # 43
#XLP5-     0.26147  -0.06141   0.55397                    # 44
#XLP6+     0.22916   0.01900   0.61649                    # 45
#XLP6-     0.16056  -0.08136   0.42321                    # 46
#XLP7+     0.23532  -0.05494   0.27204                    # 47
#XLP7-     0.30200  -0.11862   0.32735                    # 48
#END

data_NO2F_DNH_3
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.58610E+01 E(coul)=-2.47612E+01 E(vdW)=-2.10998E+01 Density= 1.88379
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_cell_length_a    5.383
_cell_length_b    6.259
_cell_length_c   10.300
_cell_angle_alpha    90.00
_cell_angle_beta     85.03
_cell_angle_gamma    90.00
_cell_formula_units_Z  2
_symmetry_space_group_name_H-M 'P 21    '
_symmetry_Int_Tables_number   4
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,-z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.38508   0.43445   0.15366                  #  1
N'2        0.56907   0.39978   0.21875                  #  2
N3         0.30691   0.62305   0.10816                  #  3
H*4        0.40332   0.75605   0.12676                  #  4
H*5        0.15569   0.62920   0.05695                  #  5
N6         0.21278   0.24870   0.11509                  #  6
O7         0.03756   0.29441   0.05180                  #  7
O8         0.26549   0.07025   0.15103                  #  8
H*9        0.58463   0.24141   0.24020                  #  9
#XC1       0.41395   0.52432   0.15409                  # 10
```

```
#XN'2      0.58377   0.43519   0.22003                    # 11
#XN3       0.28445   0.63551   0.09937                    # 12
#XH*4      0.40302   0.77745   0.12446                    # 13
#XH*5      0.19057   0.65748   0.06572                    # 14
#XN6       0.17164   0.21311   0.10498                    # 15
#XO7       0.08502   0.24236   0.07301                    # 16
#XO8       0.22115   0.11658   0.13144                    # 17
#XH*9      0.62130   0.24450   0.25215                    # 18
N1+       0.16753   0.20526   0.64968                    # 19
N'2+      0.23400   0.40952   0.70514                    # 20
O3+       0.20591   0.56990   0.64363                    # 21
O4+       0.30094   0.38952   0.81456                    # 22
N'5+      0.23231   0.16783   0.51120                    # 23
O6+       0.20410   0.31088   0.43579                    # 24
O7+       0.29811  -0.01595   0.48920                    # 25
H*8+      0.25074   0.08803   0.69965                    # 26
#XN1+     0.06072   0.21066   0.65228                    # 27
#XN'2+    0.18781   0.32813   0.70025                    # 28
#XO3+     0.26135   0.54890   0.68606                    # 29
#XO4+     0.30839   0.31370   0.77618                    # 30
#XN'5+    0.18661   0.15697   0.56291                    # 31
#XO6+     0.25915   0.23381   0.43322                    # 32
#XO7+     0.30636   0.02371   0.54348                    # 33
#XH*8+    0.26457   0.07861   0.70332                    # 34
#XLP1+    0.29355   0.25166   0.57067                    # 35
#XLP1-    0.17121   0.23770   0.62646                    # 36
#XLP2+    0.31471   0.48458   0.71412                    # 37
#XLP2-    0.15099   0.31683   0.66518                    # 38
#XLP3+    0.15267   0.43020   0.61514                    # 39
#XLP3-    0.09472   0.53438   0.78246                    # 40
#XLP4+    0.29304   0.43356   0.77899                    # 41
#XLP4-    0.27674   0.23836   0.75678                    # 42
#XLP5+    0.31249   0.16788   0.45999                    # 43
#XLP5-    0.15026   0.21222   0.58125                    # 44
#XLP6+    0.15191   0.32211   0.52841                    # 45
#XLP6-    0.09161   0.08977   0.42570                    # 46
#XLP7+    0.29037   0.05295   0.47356                    # 47
#XLP7-    0.27533   0.03637   0.59470                    # 48
#END

data_NO2F_DNH_4
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.57540E+01 E(coul)=-2.36103E+01 E(vdW)=-2.21438E+01 Density= 1.94659
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_cell_length_a    6.154
_cell_length_b    7.834
_cell_length_c   14.812
_cell_angle_alpha    90.00
_cell_angle_beta    110.43
_cell_angle_gamma    90.00
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_symmetry_space_group_name_H-M 'P 21/C  '
_symmetry_Int_Tables_number  14
loop_
_symmetry_equiv_pos_as_xyz
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  2 -x,1/2+y,1/2-z
  3 -x,-y,-z
  4 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1        0.60741   0.44260  -0.35116                    #  1
N'2       0.77202   0.47443  -0.38085                    #  2
N3        0.56318   0.51503  -0.27663                    #  3
H*4       0.67179   0.60644  -0.23836                    #  4
H*5       0.42459   0.47782  -0.26019                    #  5
N6        0.42100   0.30492  -0.40106                    #  6
O7        0.26611   0.28088  -0.36827                    #  7
O8        0.44324   0.23073  -0.46958                    #  8
H*9       0.76295   0.40028  -0.43871                    #  9
#XC1      0.64733   0.49471  -0.32188                    # 10
#XN'2     0.79081   0.49585  -0.36963                    # 11
#XN3      0.54430   0.51521  -0.27008                    # 12
#XH*4     0.67468   0.61694  -0.23071                    # 13
#XH*5     0.46095   0.50109  -0.25341                    # 14
#XN6      0.37778   0.27638  -0.40986                    # 15
#XO7      0.30220   0.26778  -0.39128                    # 16
#XO8      0.40918   0.24183  -0.44890                    # 17
#XH*9     0.79723   0.41157  -0.44107                    # 18
N1+      -0.02593   0.27853   0.84685                    # 19
N'2+     -0.13079   0.29169   0.92091                    # 20
O3+      -0.20237   0.42835   0.93506                    # 21
O4+      -0.14220   0.15357   0.95690                    # 22
N'5+      0.12766   0.41482   0.83895                    # 23
O6+       0.07462   0.56031   0.84722                    # 24
O7+       0.29139   0.36015   0.81940                    # 25
H*8+      0.06664   0.16737   0.85858                    # 26
#XN1+    -0.10464   0.28725   0.81214                    # 27
#XN'2+   -0.11354   0.26868   0.88746                    # 28
#XO3+    -0.17885   0.36685   0.95626                    # 29
#XO4+    -0.06978   0.16602   0.93748                    # 30
#XN'5+    0.06949   0.35588   0.82942                    # 31
#XO6+     0.15810   0.52738   0.84941                    # 32
#XO7+     0.24033   0.31376   0.83914                    # 33
#XH*8+    0.07924   0.15820   0.86190                    # 34
#XLP1+    0.08497   0.37556   0.88672                    # 35
#XLP1-   -0.02712   0.31756   0.85117                    # 36
#XLP2+   -0.12313   0.30445   0.96541                    # 37
#XLP2-   -0.11047   0.30720   0.86701                    # 38
```

```
#XLP3+     -0.14201   0.40933   0.88327                    # 39
#XLP3-     -0.34696   0.26650   0.91203                    # 40
#XLP4+     -0.15019   0.21231   0.95774                    # 41
#XLP4-     -0.03672   0.16059   0.90791                    # 42
#XLP5+      0.21554   0.46580   0.85802                    # 43
#XLP5-      0.00139   0.36049   0.83154                    # 44
#XLP6+     -0.02642   0.46439   0.84662                    # 45
#XLP6-      0.12848   0.49302   0.76126                    # 46
#XLP7+      0.25684   0.40623   0.82867                    # 47
#XLP7-      0.17928   0.26350   0.83941                    # 48
#END

data_NO2F_DNH_5
_chemical_name_systematic
;RAS NH3 PVDZ

E(total)=-4.56738E+01 E(coul)=-2.44896E+01 E(vdW)=-2.11843E+01 Density= 1.87976
;
_cell_length_a   20.242
_cell_length_b    5.469
_cell_length_c    6.260
_cell_angle_alpha    90.00
_cell_angle_beta     90.00
_cell_angle_gamma    90.00
_cell_formula_units_Z  4
_symmetry_space_group_name_H-M 'P 212121'
_symmetry_Int_Tables_number  19
loop_
_symmetry_equiv_pos_as_xyz
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  2 1/2+x,1/2-y,-z
  3 -x,1/2+y,1/2-z
  4 1/2-x,-y,1/2+z
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1         0.67065   0.09944   0.24708                   #  1
N'2        0.63793  -0.09317   0.28067                   #  2
N3         0.69246   0.18815   0.05845                   #  3
H*4        0.68219   0.09320  -0.07554                    #  4
H*5        0.71834   0.34557   0.05324                    #  5
N6         0.69137   0.27120   0.43445                   #  6
O7         0.72311   0.45513   0.38972                   #  7
O8         0.67433   0.20936   0.61307                   #  8
H*9        0.62809  -0.11559   0.43940                    #  9
#XC1       0.66985   0.07299   0.15677                     # 10
#XN'2      0.63705  -0.10705   0.24507                     # 11
#XN3       0.69683   0.21199   0.04609                     # 12
#XH*4      0.68321   0.09435  -0.09700                      # 13
#XH*5      0.71372   0.31043   0.02466                     # 14
```

```
#XN6       0.69671   0.31255   0.47039                 # 15
#XO7       0.71271   0.40374   0.44162                 # 16
#XO8       0.68394   0.25728   0.56688                 # 17
#XH*9      0.62202  -0.15359   0.43606                 # 18
N1+       -0.07217   0.37367   0.47338                 # 19
N'2+      -0.00192   0.32337   0.49942                 # 20
O3+        0.03472   0.36630   0.35270                 # 21
O4+        0.01111   0.25221   0.67911                 # 22
N'5+      -0.10352   0.31214   0.27077                 # 23
O6+       -0.07417   0.35426   0.10765                 # 24
O7+       -0.15934   0.23336   0.29550                 # 25
H*8+      -0.09668   0.28073   0.59073                 # 26
#XN1+     -0.07271   0.47864   0.47193                 # 27
#XN'2+    -0.02766   0.36209   0.51524                 # 28
#XO3+      0.03658   0.30873   0.42753                 # 29
#XO4+     -0.01702   0.24006   0.64277                 # 30
#XN'5+    -0.09961   0.35414   0.35332                 # 31
#XO6+     -0.09587   0.29408   0.12943                 # 32
#XO7+     -0.13893   0.22658   0.36842                 # 33
#XH*8+    -0.09853   0.26627   0.59988                 # 34
#XLP1+    -0.06808   0.25690   0.34007                 # 35
#XLP1-    -0.06625   0.37358   0.42719                 # 36
#XLP2+     0.02342   0.25017   0.49320                 # 37
#XLP2-    -0.03739   0.39849   0.46257                 # 38
#XLP3+    -0.01202   0.40798   0.34938                 # 39
#XLP3-     0.04363   0.46728   0.57672                 # 40
#XLP4+     0.01821   0.26486   0.60959                 # 41
#XLP4-    -0.04293   0.26556   0.63457                 # 42
#XLP5+    -0.10971   0.23545   0.19358                 # 43
#XLP5-    -0.08136   0.39362   0.36361                 # 44
#XLP6+    -0.05746   0.40296   0.24712                 # 45
#XLP6-    -0.14327   0.44661   0.15609                 # 46
#XLP7+    -0.14179   0.24717   0.24950                 # 47
#XLP7-    -0.12784   0.25617   0.44348                 # 48
#END
```