Supplementary Materials

Energetic tetrazoles and their rare 2*N*-oxides: Investigation of thermochemical properties

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

Ionic compounds

Ammonium NH_4 (Point group Td)

N	0.00000000	0.00000000	0.00000000
H	0.59365600	0.59365600	0.59365600
H	-0.59365600	-0.59365600	0.59365600
H	-0.59365600	0.59365600	-0.59365600
H	0.59365600	-0.59365600	-0.59365600

Hydroxylammonium NH_3OH (Point group Cs)

N	-0.04338200	-0.62718700	0.00000000
H	-1.04074200	-0.88709900	0.00000000
H	0.40103000	-1.01022700	0.85017800
H	0.40103000	-1.01022700	-0.85017800
O	-0.04338200	0.77871200	0.00000000
H	0.88940400	1.06816300	0.00000000

Hydrazinium N_2H_5 (Point group Cs)

N	0.04724100	-0.66093400	0.00000000
H	0.57178200	-0.98085800	0.82500400
H	0.57178200	-0.98085800	-0.82500400
N	0.04724100	0.78715100	0.00000000
H	-0.46227100	1.09658500	-0.82971400
H	-0.46227100	1.09658500	0.82971400
H	-0.88039300	-1.11497700	0.00000000

Guanidinium $C(NH_2)_3$ (Point group D3h)

C	0.00000000	0.00000000	0.00000000
N	0.00000000	1.33733900	0.00000000
H	0.86362100	1.86216000	0.00000000
H	-0.86362100	1.86216000	0.00000000
N	1.15817000	-0.66867000	0.00000000
H	1.18086700	-1.67899800	0.00000000
H	2.04448800	-0.18316200	0.00000000
N	-1.15817000	-0.66867000	0.00000000
H	-2.04448800	-0.18316200	0.00000000
H	-1.18086700	-1.67899800	0.00000000

Aminoguanidinium $C(NH_2)_2(NHNH_2)$ (Point group Cs)

C	0.00000000	0.50250000	0.00000000
N	-0.69193100	1.64984900	0.00000000
H	-1.70227900	1.65496400	0.00000000
H	-0.22085900	2.54334000	0.00000000
N	-0.66602400	-0.66772200	0.00000000
H	-1.68083800	-0.66950400	0.00000000

N	1.32961600	0.49684400	0.00000000
H	1.86387300	1.35367100	0.00000000
H	1.80399400	-0.39955000	0.00000000
N	0.06218700	-1.86291000	0.00000000
H	-0.15041100	-2.40517300	0.83561800
H	-0.15041100	-2.40517300	-0.83561800

Diaminoguanidinium $C(NH_2)(NHNH_2)_2$ (Point group Cs)

C	0.00000000	0.42334800	0.00000000
N	-0.66359100	-0.73941400	0.00000000
H	-0.11522300	-1.59545800	0.00000000
N	1.34779500	0.41043700	0.00000000
H	1.85920800	1.28633200	0.00000000
N	-0.66640400	1.57722200	0.00000000
H	-1.67961300	1.53894500	0.00000000
H	-0.19131000	2.46772500	0.00000000
N	2.01554100	-0.82037700	0.00000000
N	-2.06488300	-0.71966600	0.00000000
H	-2.41745400	-1.18774000	0.83292700
H	2.59131900	-0.90978100	-0.83488200
H	2.59131900	-0.90978100	0.83488200
H	-2.41745400	-1.18774000	-0.83292700

Triaminoguanidinium $C(NHNH_2)_3$ (Point group C3h)

C	0.00000000	0.00000000	0.00000000
N	0.00000000	1.34062600	0.00000000
H	-0.90095100	1.81139600	0.00000000
N	1.16101600	-0.67031300	0.00000000
H	2.01919000	-0.12545100	0.00000000
N	-1.16101600	-0.67031300	0.00000000
H	-1.11823900	-1.68594500	0.00000000
N	1.13400900	-2.07136700	0.00000000
N	1.22685200	2.01776400	0.00000000
H	1.30228500	2.59965900	0.83237300
H	1.60022800	-2.42764200	-0.83237300
H	1.60022800	-2.42764200	0.83237300
H	1.30228500	2.59965900	-0.83237300
N	-2.36086100	0.05360300	0.00000000
H	-2.90251300	-0.17201700	-0.83237300
H	-2.90251300	-0.17201700	0.83237300

5-nitrotetrazolate (Point group C2v)

C	0.00000000	0.00000000	-0.07614100
N	0.00000000	1.12347000	-0.81246400
N	0.00000000	0.67463900	-2.06202500
N	0.00000000	-0.67463900	-2.06202500
N	0.00000000	-1.12347000	-0.81246400
N	0.00000000	0.00000000	1.36171100
O	0.00000000	1.08889400	1.94798200

O	0.00000000	-1.08889400	1.94798200

5-(trinitromethyl)tetrazolate (Point group C1)

C	1.12943900	0.04851300	0.01867100
N	3.13254100	0.68793800	0.02312000
N	3.11366900	-0.64473200	0.12846900
N	1.85534800	-1.07934100	0.12153500
N	1.88798800	1.15772100	-0.04903200
C	-0.33490700	0.01451000	-0.02165100
N	-0.94060000	1.31804200	-0.58856200
O	-1.47822300	1.28848500	-1.68121900
O	-0.81152900	2.28346200	0.13867900
N	-0.82185600	-1.20709000	-0.86160300
O	-0.41931900	-1.24985900	-2.00403500
O	-1.53717000	-2.02334700	-0.30302700
N	-1.05780700	-0.15194400	1.38355700
O	-0.38328900	-0.57111100	2.29738400
O	-2.23949200	0.15458400	1.41665500

5-nitrotetrazolate 2N-oxide (Point group Cs)

C	0.00000000	0.34118200	0.00000000
N	0.68020600	-0.82452000	0.00000000
N	-0.32106400	-1.70322700	0.00000000
N	-1.55797800	-1.09421800	0.00000000
N	-1.33138000	0.20578000	0.00000000
O	-0.18091900	-2.95214500	0.00000000
N	0.64730900	1.61645300	0.00000000
O	-0.05752500	2.63481100	0.00000000
O	1.88598800	1.63621400	0.00000000

5-(trinitromethyl)tetrazolate 2N-oxide (Point group C1)

C	-0.82327000	0.24010800	-0.06825500
N	-2.70855100	1.22002400	-0.09207200
N	-2.86583700	-0.14196700	-0.05077000
N	-1.69562000	-0.78812100	-0.02699400
N	-1.40730800	1.44859700	-0.09542200
C	0.62246900	0.01771100	0.00207700
N	1.39131600	1.31933700	0.26727100
O	1.98962400	1.43823300	1.32380100
O	1.33158400	2.12884100	-0.63837200
N	0.96855300	-1.01779000	1.13122400
O	0.49309700	-0.77451700	2.21891600
O	1.65790700	-1.97618700	0.82463400
N	1.29604100	-0.58937500	-1.30253800
O	0.56997300	-1.20128000	-2.05572600
O	2.49028600	-0.37619500	-1.43723000
O	-3.98814100	-0.70162600	-0.03825300

Neutral compounds

Ammonia NH_3 (Point group C3v)

N	0.00000000	0.00000000	0.11423500
H	0.00000000	0.94525200	-0.26654800
H	-0.81861300	-0.47262600	-0.26654800
H	0.81861300	-0.47262600	-0.26654800

Hydroxylamine NH_2OH (Point group Cs)

N	0.01063600	0.70724500	0.00000000
H	-0.55593400	0.95288800	0.81454000
H	-0.55593400	0.95288800	-0.81454000
O	0.01063600	-0.73837300	0.00000000
H	0.95232800	-0.94950500	0.00000000

Hydrazine N_2H_4 (Point group C2)

N	0.00000000	0.71833000	-0.07599900
H	0.23580600	1.10106800	0.83971400
H	-0.94114300	1.02549300	-0.30771800
N	0.00000000	-0.71833000	-0.07599900
H	0.94114300	-1.02549300	-0.30771800
H	-0.23580600	-1.10106800	0.83971400

Guanidine $CNH(NH_2)_2$ (Point group C1)

C	-0.01912000	0.12111000	0.00013300
N	-0.24933100	1.38494000	0.00974500
H	-1.24922700	1.58082900	-0.04576400
N	1.28848500	-0.35557200	-0.08150100
H	1.48745900	-1.16172600	0.49990100
H	1.97116000	0.38606200	0.02074600
N	-0.95934000	-0.91203100	0.07616400
H	-1.91858600	-0.61346600	-0.04202300
H	-0.73478200	-1.73972000	-0.46451600

Aminoguanidine $C(NH_2)_2(NNH_2)$ (Point group C1)

C	-0.42374500	-0.04091000	0.00031800
N	-1.69182400	-0.61647900	-0.07859700
H	-2.36709500	-0.20785200	0.55892500
N	0.61852900	-0.80685400	0.01612400
N	-0.41340400	1.34230300	0.05991200
H	-1.16658500	1.78862900	-0.45009900
H	0.51093700	1.71042300	-0.15451600
N	1.84455000	-0.03704100	-0.04870400
H	2.19232600	0.04999900	0.90916800
H	2.51627900	-0.64308200	-0.51596800
H	-1.64835000	-1.62616100	0.00943500

Diaminoguanidine $C(NH_2)(NHNH_2)(NNH_2)$ (Point group C1)

C	-0.03763300	0.33546500	-0.01358200
N	-0.57909900	-0.83784800	-0.01329700
N	1.35338900	0.46486700	-0.06360200

H	1.70302700	1.19990000	0.54117700
N	-0.72001900	1.54198100	0.05946200
N	2.15134400	-0.70166100	0.05599200
N	-2.01934400	-0.76486800	-0.05613700
H	-2.35733300	-0.68200600	0.90638900
H	1.64451600	-1.38304100	0.62777900
H	2.21230400	-1.11646200	-0.87237700
H	-2.32560600	-1.68302700	-0.36887000
H	-0.25998600	2.30746800	-0.42074400
H	-1.69502300	1.42708000	-0.20879000

Triaminoguanidine $C(NHNH_2)_2(NNH_2)$ (Point group C1)

C	-0.04731500	0.06813800	0.00022700
N	-0.36661700	1.32289300	0.08150800
N	0.80195900	2.17116500	0.06850800
N	1.26130800	-0.37451200	-0.18568400
N	1.51755700	-1.74721000	0.05638100
N	-1.02747200	-0.90170600	0.08058300
N	-2.38224000	-0.53516500	-0.08103700
H	0.47152200	3.08310700	0.37296600
H	1.09813100	2.29816400	-0.90383900
H	1.92168400	0.30215800	0.19772600
H	2.27234800	-2.04230200	-0.55565200
H	1.79146700	-1.90740700	1.02566300
H	-0.78737800	-1.79958100	-0.31695700
H	-2.68570100	-0.11956000	0.79902100
H	-2.42965300	0.22833500	-0.76210700

5-nitrotetrazole (Point group Cs)

C	0.00000000	0.03507100	0.00000000
N	1.00050900	0.94539800	0.00000000
N	0.40856400	2.11032900	0.00000000
N	-0.90167200	1.84920700	0.00000000
N	-1.21531700	0.56706500	0.00000000
N	0.22614500	-1.41127700	0.00000000
O	1.39119500	-1.78017000	0.00000000
O	-0.76937400	-2.12226600	0.00000000
H	-1.60216900	2.58400400	0.00000000

5-(trinitromethyl)tetrazole (Point group C1)

C	1.08727400	0.04483400	0.01202300
N	3.04211400	0.61429000	-0.02538700
N	3.07253800	-0.71290400	0.09331600
N	1.82623200	-1.09253400	0.11626500
N	1.83159900	1.14112200	-0.08300900
C	-0.40031100	0.01217000	-0.00327300
N	-1.01464600	1.34020300	-0.50491500
O	-1.66791500	1.31191900	-1.52561500
O	-0.77351400	2.29078600	0.21242600
N	-0.87935600	-1.14607400	-0.92791600

O	-0.34633900	-1.16139000	-2.01790600
O	-1.71997200	-1.90039400	-0.48673000
N	-1.02767500	-0.23297100	1.40619200
O	-0.30510600	-0.76839600	2.22098000
O	-2.18261100	0.11553100	1.53406800
H	3.88622800	1.17559900	-0.07210600

5-nitrotetrazole 2N-oxide (Point group Cs)

C	0.00000000	0.39019300	0.00000000
N	0.68503100	-0.76162500	0.00000000
N	-0.31781800	-1.59415400	0.00000000
N	-1.53610700	-1.06338700	0.00000000
N	-1.33275500	0.24079800	0.00000000
O	-0.09853400	-2.93160700	0.00000000
H	-0.99125000	-3.32311800	0.00000000
N	0.66564500	1.69136400	0.00000000
O	-0.06046500	2.67453800	0.00000000
O	1.88940900	1.68094300	0.00000000

5-(trinitromethyl)tetrazole 2N-oxide (Point group C1)

C	-0.77721400	0.23471400	-0.06848900
N	-2.65759800	1.22724800	-0.09475100
N	-2.77180400	-0.09285500	-0.03919000
N	-1.66277000	-0.77457600	-0.01590300
N	-1.35838800	1.44953400	-0.10894400
C	0.68936200	-0.00285100	-0.01098000
N	1.46237700	1.33090400	0.11861400
O	2.08217900	1.52053600	1.14390700
O	1.36099600	2.05284100	-0.85110900
N	1.03925400	-0.89588800	1.22247500
O	0.43749600	-0.60562900	2.23580900
O	1.86758000	-1.76654400	1.06033200
N	1.27475500	-0.72733700	-1.26414800
O	0.50529800	-1.45240400	-1.86100900
O	2.44717100	-0.52008200	-1.49454200
O	-3.96676100	-0.72873900	-0.01155200
H	-4.62534500	-0.01023100	-0.02494400

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 method.

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

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

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

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

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 5 polymorphs of Ammonium 5-nitrotetrazolate (ionic form).

data_T_NH4_1

_symmetry_cell_setting orthorhombic

```
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.111
_cell_length_b                 9.953
_cell_length_c                 8.678
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1046.05
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.64910 -0.04129 0.62869
H*2 H 0.64462 -0.02578 0.74561
H*3 H 0.58733 -0.10587 0.59537
H*4 H 0.63996 0.04883 0.57229
H*5 H 0.72449 -0.08235 0.60149
C1+ C 0.48554 -0.16174 0.11807
N'2+ N 0.39734 -0.08368 0.08988
N'3+ N 0.33654 -0.15768 -0.00501
N'4+ N 0.38745 -0.27595 -0.03197
N'5+ N 0.48212 -0.28064 0.04499
N6+ N 0.57498 -0.12187 0.21695
O7+ O 0.57037 -0.01016 0.27902
O8+ O 0.65254 -0.20106 0.23551

#END

data_T_NH4_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P c a 21'
_symmetry_Int_Tables_number      29
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.332
_cell_length_b                 5.459
_cell_length_c                 7.662
_cell_angle_alpha               90.00
_cell_angle_beta               90.00
_cell_angle_gamma                 90.00
_cell_volume                   515.809
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.12584 0.19459 0.17404
H*2 H -0.16887 0.35584 0.17264
H*3 H -0.13622 0.10919 0.29242
H*4 H -0.15335 0.08217 0.07596
H*5 H -0.04493 0.23116 0.15513
C1+ C 0.14953 0.38700 0.14775
N'2+ N 0.25448 0.38165 0.10096
N'3+ N 0.26104 0.18545 -0.00091
N'4+ N 0.16277 0.07826 -0.01377
N'5+ N 0.09084 0.20314 0.07954
N6+ N 0.10437 0.57174 0.26005
O7+ O 0.16526 0.73357 0.31621
O8+ O 0.00666 0.56055 0.29545

#END

data_T_NH4_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 10.096
_cell_length_b                 10.904
_cell_length_c                 17.459
_cell_angle_alpha               90.00
_cell_angle_beta               128.34
_cell_angle_gamma                 90.00
_cell_volume                   1507.51
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.25639 0.62034 0.61671
H*2 H 0.35923 0.63270 0.61852
H*3 H 0.25576 0.53192 0.63688
H*4 H 0.26300 0.68054 0.66428
H*5 H 0.14756 0.63619 0.54715
C1+ C 0.22502 0.34699 0.72397
N'2+ N 0.13846 0.25100 0.72091
N'3+ N 0.00220 0.24631 0.62782
N'4+ N 0.00830 0.33694 0.57746
N'5+ N 0.14861 0.40193 0.63705
N6+ N 0.38415 0.38709 0.81182
O7+ O 0.44411 0.33029 0.88828
O8+ O 0.45395 0.47657 0.80700

#END

data_T_NH4_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C c'
_symmetry_Int_Tables_number      9
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.700
_cell_length_b                 6.437
_cell_length_c                 7.837
_cell_angle_alpha               90.00
_cell_angle_beta                50.30
_cell_angle_gamma                 90.00
_cell_volume                   492.934
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.46800 0.16971 0.53267
H*2 H 0.45891 0.25368 0.43111
H*3 H 0.39066 0.06177 0.61912
H*4 H 0.56098 0.09509 0.43815
H*5 H 0.46144 0.26830 0.64229
C1+ C 0.22640 0.27497 0.29456
```

```
N'2+ N 0.21466 0.47771 0.34454
N'3+ N 0.31402 0.50931 0.35429
N'4+ N 0.38235 0.33033 0.31129
N'5+ N 0.32845 0.17965 0.27293
N6+ N 0.13822 0.17009 0.26688
O7+ O 0.04712 0.27177 0.29030
O8+ O 0.15741 -0.01711 0.22089

#END

data_T_NH4_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.648
_cell_length_b                 5.582
_cell_length_c                 12.679
_cell_angle_alpha               90.00
_cell_angle_beta                75.22
_cell_angle_gamma                 90.00
_cell_volume                   523.371
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.79768 0.08472 0.38673
H*2 H 0.77814 -0.07564 0.42791
H*3 H 0.77057 0.06400 0.31192
H*4 H 0.71249 0.21175 0.43106
H*5 H 0.92952 0.13877 0.37603
C1+ C 0.71736 0.09618 0.12214
N'2+ N 0.80988 -0.04155 0.17598
N'3+ N 0.87244 -0.21787 0.10629
N'4+ N 0.81834 -0.18498 0.01402
N'5+ N 0.71978 0.01322 0.02233
N6+ N 0.62466 0.31165 0.16702
O7+ O 0.63052 0.37297 0.25978
O8+ O 0.54319 0.42605 0.11086

#END
```

S7. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylammonium 5-nitrotetrazolate (ionic form).

```
data_T_NH3OH_1
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.753
_cell_length_b                 13.366
_cell_length_c                 10.636
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1102.17
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.40080 0.14985 0.41466
H*2 H 0.45429 0.19563 0.34712
H*3 H 0.40120 0.07709 0.38193
H*4 H 0.47238 0.15588 0.49622
O5 O 0.23218 0.18641 0.43066
H*6 H 0.17659 0.14480 0.49435
C1+ C 0.10102 0.45177 0.18726
N'2+ N 0.05635 0.45912 0.30893
N'3+ N -0.00223 0.36836 0.33636
N'4+ N 0.00763 0.30923 0.23379
N'5+ N 0.07278 0.36065 0.13812
N6+ N 0.17221 0.53357 0.11643
O7+ O 0.19327 0.61464 0.17033
O8+ O 0.20920 0.51921 0.00478

#END

data_T_NH3OH_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.377
_cell_length_b                 11.708
_cell_length_c                 6.437
_cell_angle_alpha               90.00
_cell_angle_beta                115.70
_cell_angle_gamma                90.00
_cell_volume                   568.875
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.29429 0.40444 -0.33799
H*2 H 0.17656 0.39157 -0.48209
H*3 H 0.29100 0.48375 -0.26967
H*4 H 0.30986 0.34064 -0.21988
O5 O 0.42484 0.39873 -0.41975
H*6 H 0.53925 0.41058 -0.28769
C1+ C 0.45619 0.21363 0.14834
N'2+ N 0.48771 0.11139 0.25328
N'3+ N 0.35810 0.04620 0.10674
N'4+ N 0.25321 0.10825 -0.07921
N'5+ N 0.31303 0.21472 -0.05639
N6+ N 0.56518 0.31239 0.24577
O7+ O 0.69427 0.30259 0.43557
O8+ O 0.52497 0.40274 0.13543

#END

data_T_NH3OH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 14.992
_cell_length_b                 6.960
_cell_length_c                 5.924
_cell_angle_alpha               90.00
_cell_angle_beta                64.40
_cell_angle_gamma                90.00
_cell_volume                   557.455
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.14582 0.27198 0.22074
H*2 H -0.21697 0.30264 0.24754
H*3 H -0.13542 0.12503 0.20389
H*4 H -0.09686 0.34111 0.06080
O5 O -0.14011 0.34316 0.43620
H*6 H -0.07338 0.31683 0.41825
C1+ C 0.09549 0.25203 0.39122
N'2+ N 0.00014 0.24110 0.55786
N'3+ N 0.00320 0.13988 0.74434
N'4+ N 0.09765 0.09253 0.68917
N'5+ N 0.15743 0.16224 0.46599
N6+ N 0.12812 0.35038 0.15553
O7+ O 0.06520 0.42869 0.10395
O8+ O 0.21765 0.35227 0.01491

#END

data_T_NH3OH_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 13.177
_cell_length_b                 7.065
_cell_length_c                 10.143
_cell_angle_alpha               90.00
_cell_angle_beta                33.56
_cell_angle_gamma                 90.00
_cell_volume                   522.001
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.24870 -0.68145 0.71713
H*2 H 0.16427 -0.77216 0.75699
H*3 H 0.35888 -0.75721 0.63425
H*4 H 0.29263 -0.57554 0.60684
O5 O 0.13757 -0.61002 0.93926
```

```
H*6 H 0.21287 -0.52282 0.90931
C1+ C 0.73023 0.23920 -0.00561
N'2+ N 0.69892 0.42527 0.04368
N'3+ N 0.58698 0.46693 0.06572
N'4+ N 0.55329 0.30991 0.03043
N'5+ N 0.64282 0.16379 -0.01509
N6+ N 0.84614 0.13116 -0.04448
O7+ O 0.92059 0.21383 -0.03185
O8+ O 0.86621 -0.03961 -0.08880

#END

data_T_NH3OH_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.972
_cell_length_b                 10.952
_cell_length_c                 6.404
_cell_angle_alpha               90.00
_cell_angle_beta                79.10
_cell_angle_gamma                90.00
_cell_volume                   549.042
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.24249 0.08314 -0.19746
H*2 H 0.18397 0.14893 -0.09356
H*3 H 0.14955 0.03044 -0.24620
H*4 H 0.31797 0.12566 -0.32576
O5 O 0.34057 0.01487 -0.07848
H*6 H 0.39853 -0.04892 -0.17173
C1+ C 0.11252 -0.17164 -0.44539
N'2+ N 0.04462 -0.11374 -0.26418
N'3+ N -0.05041 -0.19909 -0.15134
N'4+ N -0.03884 -0.30426 -0.26287
N'5+ N 0.06389 -0.28889 -0.44990
N6+ N 0.22630 -0.11369 -0.61793
O7+ O 0.26335 -0.00519 -0.59827
O8+ O 0.28203 -0.17494 -0.77828

#END
```

S8. Optimized crystal structure coordinates for 5 polymorphs of Hydrazinium 5-nitrotetrazolate (ionic form).

```
data_T_N2H5_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 5.549
_cell_length_b                 8.638
_cell_length_c                 14.329
_cell_angle_alpha               90.00
_cell_angle_beta               124.53
_cell_angle_gamma                90.00
_cell_volume                   565.824
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.06834 0.14582 -0.35562
H*2 H -0.02760 0.06166 -0.39577
H*3 H -0.08851 0.09007 -0.29694
N4 N -0.34672 0.21706 -0.43867
H*5 H -0.38708 0.29924 -0.39789
H*6 H -0.32582 0.27066 -0.49729
H*7 H 0.10951 0.21937 -0.31352
C1+ C 0.20140 -0.36972 0.63946
N'2+ N 0.17925 -0.47931 0.70073
N'3+ N 0.30394 -0.60208 0.68904
N'4+ N 0.39691 -0.56586 0.62278
N'5+ N 0.33407 -0.41901 0.59039
N6+ N 0.09350 -0.21460 0.62755
O7+ O -0.02552 -0.18058 0.67617
O8+ O 0.12453 -0.12212 0.56923

#END

data_T_N2H5_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 5.638
_cell_length_b 8.722
_cell_length_c 12.077
_cell_angle_alpha 90.00
_cell_angle_beta 103.91
_cell_angle_gamma 90.00
_cell_volume 576.466
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.38191 0.82964 0.65773
H*2 H 0.27769 0.92408 0.62674
H*3 H 0.51619 0.86664 0.72607
N4 N 0.49832 0.77635 0.57023
H*5 H 0.60354 0.68367 0.60211
H*6 H 0.36367 0.74144 0.50222
H*7 H 0.27334 0.75094 0.68632
C1+ C 0.05264 0.15482 0.13455
N'2+ N 0.21650 0.04932 0.18537
N'3+ N 0.08707 -0.07932 0.17473
N'4+ N -0.14636 -0.05045 0.11923
N'5+ N -0.17223 0.09740 0.09295
N6+ N 0.11223 0.31390 0.12555
O7+ O 0.32490 0.35546 0.16668
O8+ O -0.05186 0.40207 0.07710

#END

data_T_N2H5_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 8.442
_cell_length_b 12.528
_cell_length_c 5.598
_cell_angle_alpha 90.00
_cell_angle_beta 95.47
_cell_angle_gamma 90.00

```
_cell_volume                    589.356
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.26929 0.60101 0.27985
H*2 H 0.31927 0.53365 0.21346
H*3 H 0.35449 0.63444 0.40075
N4 N 0.13687 0.56824 0.40922
H*5 H 0.08905 0.63543 0.47680
H*6 H 0.05362 0.53407 0.28844
H*7 H 0.24300 0.65409 0.14053
C1+ C 0.18450 -0.16403 0.92147
N'2+ N 0.13878 -0.26663 0.90268
N'3+ N 0.02302 -0.26541 0.72466
N'4+ N 0.00115 -0.16497 0.64095
N'5+ N 0.10236 -0.09937 0.76328
N6+ N 0.30933 -0.12700 1.09428
O7+ O 0.37788 -0.19295 1.23229
O8+ O 0.34258 -0.03083 1.09718

#END

data_T_N2H5_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  7.317
_cell_length_b                  8.297
_cell_length_c                  14.400
_cell_angle_alpha                 90.00
_cell_angle_beta                 42.14
_cell_angle_gamma                   90.00
_cell_volume                    586.548
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.99426 0.35802 -0.13483
H*2 H 0.97359 0.48138 -0.12829
H*3 H 1.08146 0.32554 -0.22989
```

N4 N 0.72452 0.28777 -0.02906
H*5 H 0.74669 0.16533 -0.03725
H*6 H 0.63821 0.32206 0.06493
H*7 H 1.12537 0.32713 -0.13105
C1+ C 0.25366 0.37627 0.44948
N'2+ N 0.23682 0.43726 0.54205
N'3+ N 0.13444 0.31639 0.62995
N'4+ N 0.09216 0.18786 0.59032
N'5+ N 0.16641 0.22322 0.47605
N6+ N 0.35529 0.46616 0.33316
O7+ O 0.43085 0.60654 0.31772
O8+ O 0.36260 0.39909 0.25375

#END

data_T_N2H5_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.658
_cell_length_b 8.505
_cell_length_c 8.554
_cell_angle_alpha 90.00
_cell_angle_beta 80.51
_cell_angle_gamma 90.00
_cell_volume 549.508
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.79927 0.02374 0.86145
H*2 H 0.78675 -0.09206 0.89617
H*3 H 0.91721 0.03279 0.78458
N4 N 0.81197 0.11826 0.99993
H*5 H 0.82636 0.23280 0.96415
H*6 H 0.69516 0.10723 1.07638
H*7 H 0.69712 0.05156 0.80119
C1+ C 0.31577 0.14149 0.46822
N'2+ N 0.20587 0.19698 0.59488
N'3+ N 0.11619 0.07047 0.65283
N'4+ N 0.17166 -0.05594 0.56290
N'5+ N 0.29824 -0.01353 0.44511
N6+ N 0.44019 0.23867 0.36711

O7+ O 0.44616 0.38031 0.39846
O8+ O 0.53569 0.17628 0.25330

#END

S9. Optimized crystal structure coordinates for 5 polymorphs of Guanidinium 5-nitrotetrazolate (ionic form).

```
data_T_GH_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.269
_cell_length_b                 11.301
_cell_length_c                 7.455
_cell_angle_alpha               90.00
_cell_angle_beta                56.18
_cell_angle_gamma                 90.00
_cell_volume                   648.767
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74996 0.88723 0.75001
N2 N 0.74991 0.76889 0.75007
H*3 H 0.84326 0.72244 0.74966
H*4 H 0.65652 0.72246 0.75054
N5 N 0.87520 0.94638 0.74939
H*6 H 0.87769 1.03579 0.74933
H*7 H 0.97100 0.90341 0.74896
N8 N 0.62477 0.94642 0.75057
H*9 H 0.52893 0.90347 0.75104
H*10 H 0.62236 1.03582 0.75053
C1+ C 0.24995 0.87081 -0.24994
N'2+ N 0.37594 0.80565 -0.26115
N'3+ N 0.32559 0.69508 -0.25663
N'4+ N 0.17426 0.69508 -0.24314
N'5+ N 0.12394 0.80565 -0.23869
N6+ N 0.24997 0.99804 -0.24998
O7+ O 0.37210 1.04992 -0.26088
O8+ O 0.12785 1.04992 -0.23911

#END
```

```
data_T_GH_2
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                  7.297
_cell_length_b                  36.211
_cell_length_c                  7.311
_cell_angle_alpha                140.75
_cell_angle_beta                 78.76
_cell_angle_gamma                138.40
_cell_volume                    328.245
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.79513 -0.24726 -0.04578
N2 N -0.64245 -0.23569 0.11112
H*3 H -0.48051 -0.22850 0.08881
H*4 H -0.68456 -0.23379 0.25658
N5 N -0.73466 -0.24949 -0.23673
H*6 H -0.84732 -0.25816 -0.35748
H*7 H -0.57452 -0.24257 -0.26586
N8 N -1.00830 -0.25659 -0.01174
H*9 H -1.05757 -0.25511 0.13131
H*10 H -1.12633 -0.26540 -0.12807
C1+ C -0.27713 0.75279 -0.53030
N'2+ N -0.35150 0.74654 -0.36426
N'3+ N -0.21801 0.73803 -0.33071
N'4+ N -0.06923 0.73924 -0.47290
N'5+ N -0.10375 0.74855 -0.60105
N6+ N -0.37380 0.76304 -0.62333
O7+ O -0.53328 0.76625 -0.54651
O8+ O -0.29315 0.76819 -0.77601

#END

data_T_GH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.299
_cell_length_b                 12.443
_cell_length_c                 9.271
_cell_angle_alpha               90.00
_cell_angle_beta                129.27
_cell_angle_gamma                 90.00
_cell_volume                   651.857
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.78156 0.12355 0.03130
N2 N 0.54500 0.12034 -0.08591
H*3 H 0.45294 0.11831 -0.03837
H*4 H 0.45140 0.11984 -0.22544
N5 N 0.90088 0.12413 0.21534
H*6 H 1.07961 0.12654 0.30635
H*7 H 0.81579 0.12218 0.26878
N8 N 0.89880 0.12618 -0.03553
H*9 H 0.81213 0.12580 -0.17408
H*10 H 1.07749 0.12863 0.05056
C1+ C 0.74870 0.12428 0.51393
N'2+ N 0.61789 0.13064 0.56942
N'3+ N 0.39699 0.13003 0.41053
N'4+ N 0.39762 0.12348 0.26556
N'5+ N 0.61893 0.11975 0.32801
N6+ N 1.00312 0.12248 0.64128
O7+ O 1.10635 0.12703 0.81019
O8+ O 1.10736 0.11647 0.57621

#END

data_T_GH_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C c'
_symmetry_Int_Tables_number      9
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 11.302
_cell_length_b                 9.270
_cell_length_c                 7.576
_cell_angle_alpha               90.00
_cell_angle_beta                55.23
```

```
_cell_angle_gamma               90.00
_cell_volume                   652.011
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.31385 0.14167 0.26300
N2 N 0.25169 0.26634 0.27019
H*3 H 0.16060 0.26843 0.27471
H*4 H 0.29400 0.36209 0.27131
N5 N 0.25548 0.01653 0.26168
H*6 H 0.30069 -0.07888 0.25629
H*7 H 0.16447 0.01373 0.26604
N8 N 0.43437 0.14214 0.25713
H*9 H 0.48026 0.23546 0.25800
H*10 H 0.48309 0.04918 0.25165
C1+ C 0.33003 0.35889 -0.23620
N'2+ N 0.39908 0.23797 -0.24611
N'3+ N 0.50784 0.28643 -0.24152
N'4+ N 0.50302 0.43175 -0.22926
N'5+ N 0.39105 0.47996 -0.22568
N6+ N 0.20304 0.35874 -0.23678
O7+ O 0.15515 0.24141 -0.24692
O8+ O 0.14737 0.47596 -0.22712

#END

data_T_GH_5
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 6.433
_cell_length_b                 7.310
_cell_length_c                 7.307
_cell_angle_alpha               78.74
_cell_angle_beta                96.28
_cell_angle_gamma              103.54
_cell_volume                   326.902
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24649 -0.20529 0.53939
```

N2 N 0.24712 -0.02142 0.47196
H*3 H 0.24353 0.02922 0.33296
H*4 H 0.25122 0.07224 0.55805
N5 N 0.24102 -0.32607 0.42217
H*6 H 0.24044 -0.46554 0.47015
H*7 H 0.23731 -0.28139 0.28219
N8 N 0.25133 -0.26838 0.72404
H*9 H 0.25550 -0.17955 0.81506
H*10 H 0.25095 -0.40672 0.77793
C1+ C 0.24924 0.28001 0.02182
N'2+ N 0.25464 0.09471 0.07711
N'3+ N 0.25826 0.03431 -0.08225
N'4+ N 0.25510 0.17985 -0.22729
N'5+ N 0.24936 0.33707 -0.16443
N6+ N 0.24385 0.40521 0.14967
O7+ O 0.24421 0.33881 0.31886
O8+ O 0.23910 0.57371 0.08475

#END

S10. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidinium 5-nitrotetrazolate (ionic form).

data_T_AGH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 8.029
_cell_length_b 19.850
_cell_length_c 8.764
_cell_angle_alpha 90.00
_cell_angle_beta 148.20
_cell_angle_gamma 90.00
_cell_volume 736.035
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.01808 0.33803 0.70728
N2 N 0.05172 0.28662 0.85478
H*3 H 0.13904 0.29457 1.02854
H*4 H 0.01886 0.23839 0.79609
N5 N 0.02920 0.40160 0.79258
H*6 H 0.11684 0.40993 0.96693

N7 N -0.13297 0.32752 0.47863
H*8 H -0.17162 0.28059 0.40817
H*9 H -0.18179 0.36822 0.37477
N10 N -0.04416 0.45510 0.63765
H*11 H -0.21423 0.48479 0.55259
H*12 H 0.15315 0.48276 0.76875
C1+ C 0.08664 -0.11523 0.38474
N'2+ N 0.18305 -0.07018 0.56428
N'3+ N 0.26446 -0.10817 0.74599
N'4+ N 0.21737 -0.17373 0.67555
N'5+ N 0.10464 -0.17935 0.44697
N6+ N -0.02505 -0.09660 0.14867
O7+ O -0.03260 -0.03611 0.10927
O8+ O -0.10859 -0.14191 -0.00443

#END

data_T_AGH_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 4.128
_cell_length_b 20.341
_cell_length_c 11.319
_cell_angle_alpha 90.00
_cell_angle_beta 52.45
_cell_angle_gamma 90.00
_cell_volume 753.521
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.76516 0.63700 0.79781
N2 N 0.76693 0.69393 0.73788
H*3 H 0.75883 0.69498 0.65047
H*4 H 0.77645 0.73747 0.77858
N5 N 0.75230 0.58001 0.74025
H*6 H 0.74411 0.58072 0.65245
N7 N 0.77583 0.63567 0.91284
H*8 H 0.78562 0.67736 0.95901
H*9 H 0.77390 0.59124 0.95393
N10 N 0.75051 0.52070 0.80332
H*11 H 0.49017 0.49506 0.84364

```
H*12 H 1.00047 0.49337 0.72627
C1+ C 0.21411 0.36292 -0.31500
N'2+ N 0.21953 0.41585 -0.38717
N'3+ N 0.23752 0.39009 -0.49883
N'4+ N 0.24256 0.32388 -0.49263
N'5+ N 0.22792 0.30560 -0.37685
N6+ N 0.19533 0.36722 -0.18415
O7+ O 0.18361 0.42240 -0.13580
O8+ O 0.19174 0.31555 -0.12579

#END

data_T_AGH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.994
_cell_length_b                 12.453
_cell_length_c                 7.618
_cell_angle_alpha               90.00
_cell_angle_beta                77.53
_cell_angle_gamma                90.00
_cell_volume                   740.476
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.06489 -0.24697 0.73062
N2 N 0.03677 -0.16750 0.62197
H*3 H -0.01557 -0.18201 0.51486
H*4 H 0.06722 -0.09072 0.64427
N5 N 0.02246 -0.34827 0.69622
H*6 H -0.03016 -0.36338 0.58885
N7 N 0.13377 -0.22780 0.87154
H*8 H 0.16725 -0.15295 0.90166
H*9 H 0.15231 -0.29087 0.94942
N10 N 0.05214 -0.43094 0.81019
H*11 H -0.06029 -0.46723 0.86870
H*12 H 0.13520 -0.48569 0.74013
C1+ C 0.17589 0.19293 -0.24102
N'2+ N 0.24892 0.14404 -0.11934
N'3+ N 0.22860 0.04035 -0.14963
N'4+ N 0.14595 0.02849 -0.28526
```

N'5+ N 0.11130 0.12428 -0.34521
N6+ N 0.16765 0.30770 -0.25809
O7+ O 0.23098 0.36407 -0.15559
O8+ O 0.09759 0.34492 -0.37450

#END

data_T_AGH_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.349
_cell_length_b 6.909
_cell_length_c 14.889
_cell_angle_alpha 90.00
_cell_angle_beta 98.55
_cell_angle_gamma 90.00
_cell_volume 747.576
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.42079 0.64515 0.09546
N2 N 0.41716 0.74511 0.01810
H*3 H 0.53341 0.77186 -0.00846
H*4 H 0.29775 0.79657 -0.01587
N5 N 0.58285 0.57902 0.13866
H*6 H 0.70012 0.60540 0.11234
N7 N 0.26772 0.61002 0.13035
H*8 H 0.14369 0.65722 0.09993
H*9 H 0.27821 0.53365 0.18906
N10 N 0.58578 0.47469 0.21944
H*11 H 0.63500 0.33862 0.21230
H*12 H 0.66458 0.54447 0.27162
C1+ C 0.03571 0.15299 0.11595
N'2+ N -0.04667 0.22058 0.03547
N'3+ N 0.09252 0.25027 -0.01041
N'4+ N 0.25234 0.20157 0.04153
N'5+ N 0.21947 0.13949 0.12198
N6+ N -0.06328 0.10019 0.18863
O7+ O -0.23262 0.11796 0.17634
O8+ O 0.02533 0.03936 0.26019

#END

data_T_AGH_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.257
_cell_length_b 14.476
_cell_length_c 7.445
_cell_angle_alpha 90.00
_cell_angle_beta 106.19
_cell_angle_gamma 90.00
_cell_volume 751.098
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.03636 0.59339 0.13479
N2 N 0.09089 0.51719 0.23808
H*3 H 0.22271 0.48954 0.25644
H*4 H 0.00145 0.48522 0.30057
N5 N 0.15993 0.63392 0.05382
H*6 H 0.29253 0.60650 0.07172
N7 N -0.13713 0.62972 0.11071
H*8 H -0.23369 0.60130 0.16916
H*9 H -0.17109 0.68746 0.03119
N10 N 0.10215 0.71350 -0.05390
H*11 H 0.18909 0.76758 0.00199
H*12 H 0.10464 0.70220 -0.18825
C1+ C 0.52761 0.11398 0.85834
N'2+ N 0.46356 0.03221 0.78028
N'3+ N 0.61983 -0.00721 0.75540
N'4+ N 0.77161 0.04970 0.81704
N'5+ N 0.71632 0.12698 0.88292
N6+ N 0.40590 0.18112 0.91056
O7+ O 0.23378 0.16257 0.88210
O8+ O 0.47875 0.25442 0.98159

#END

S11. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidinium 5-nitrotetrazolate (ionic form).
data_T_DAGH_1

```
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                  8.678
_cell_length_b                  8.520
_cell_length_c                  6.677
_cell_angle_alpha                106.65
_cell_angle_beta                117.22
_cell_angle_gamma                82.85
_cell_volume                    420.585
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.49692 0.78110 0.49100
N2 N 0.64633 0.73576 0.47860
H*3 H 0.64376 0.70367 0.31826
N4 N 0.35147 0.78228 0.29325
H*5 H 0.23767 0.81644 0.30090
N6 N 0.49248 0.82445 0.69652
H*7 H 0.60502 0.82173 0.84069
H*8 H 0.38165 0.85913 0.71085
N9 N 0.36088 0.73598 0.08030
N10 N 0.79713 0.73479 0.68481
H*11 H 0.88662 0.81336 0.70763
H*12 H 0.28420 0.63611 -0.02745
H*13 H 0.32444 0.83043 0.00334
H*14 H 0.84648 0.61950 0.67691
C1+ C 0.08442 0.19685 0.77202
N'2+ N 0.23896 0.12783 0.80377
N'3+ N 0.21816 -0.02436 0.80222
N'4+ N 0.05600 -0.04444 0.77047
N'5+ N -0.03107 0.09439 0.75090
N6+ N 0.04629 0.36429 0.76164
O7+ O 0.16160 0.44877 0.78303
O8+ O -0.10012 0.41635 0.73179

#END

data_T_DAGH_2
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
```

```
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 8.689
_cell_length_b                 8.414
_cell_length_c                 7.064
_cell_angle_alpha               108.53
_cell_angle_beta                62.37
_cell_angle_gamma                 90.78
_cell_volume                   428.292
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74923 0.49628 -0.01149
N2 N 0.71114 0.64235 0.16126
H*3 H 0.67416 0.63600 0.31759
N4 N 0.73714 0.34907 0.02852
H*5 H 0.76574 0.23777 -0.10129
N6 N 0.79844 0.49685 -0.22017
H*7 H 0.80572 0.61054 -0.24235
H*8 H 0.82790 0.38862 -0.35340
N9 N 0.68503 0.35320 0.24990
N10 N 0.72394 0.79501 0.11862
H*11 H 0.81411 0.85502 0.15636
H*12 H 0.57169 0.30378 0.31028
H*13 H 0.78172 0.28739 0.25133
H*14 H 0.60457 0.87137 0.21517
C1+ C 0.18079 0.09352 0.30392
N'2+ N 0.23715 0.23852 0.37532
N'3+ N 0.38487 0.18575 0.36550
N'4+ N 0.41472 0.01455 0.29046
N'5+ N 0.28685 -0.04657 0.25037
N6+ N 0.02223 0.08872 0.28651
O7+ O -0.06651 0.22492 0.33996
O8+ O -0.01834 -0.05140 0.21885

#END

data_T_DAGH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.627
_cell_length_b                 8.550
_cell_length_c                 16.865
_cell_angle_alpha               90.00
_cell_angle_beta                69.38
_cell_angle_gamma                 90.00
_cell_volume                   1704.12
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25670 0.48362 0.50048
N2 N 0.16955 0.50632 0.57286
H*3 H 0.09023 0.50150 0.57057
N4 N 0.23592 0.45574 0.42866
H*5 H 0.30140 0.43840 0.37353
N6 N 0.36255 0.48860 0.49967
H*7 H 0.37417 0.50993 0.55518
H*8 H 0.42978 0.47191 0.44602
N9 N 0.12364 0.45132 0.43184
N10 N 0.19168 0.53526 0.64733
H*11 H 0.15541 0.45052 0.69087
H*12 H 0.11021 0.53593 0.39396
H*13 H 0.10533 0.34416 0.41367
H*14 H 0.16028 0.64184 0.67121
C1+ C 0.40490 0.44236 0.20137
N'2+ N 0.36317 0.34746 0.26871
N'3+ N 0.37982 0.20535 0.23480
N'4+ N 0.42993 0.21620 0.14991
N'5+ N 0.44661 0.36553 0.12734
N6+ N 0.40492 0.61004 0.20789
O7+ O 0.36449 0.66965 0.27906
O8+ O 0.44536 0.68717 0.14205

#END

data_T_DAGH_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.637
_cell_length_b                 8.458
_cell_length_c                 8.231
_cell_angle_alpha               90.00
_cell_angle_beta                71.41
_cell_angle_gamma                 90.00
_cell_volume                   833.858
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.75229 0.33574 0.49492
N2 N 0.67131 0.31329 0.64427
H*3 H 0.59196 0.30051 0.64128
N4 N 0.72561 0.34039 0.34896
H*5 H 0.78640 0.35734 0.23520
N6 N 0.85787 0.35324 0.49104
H*7 H 0.87406 0.34892 0.60395
H*8 H 0.92052 0.37031 0.38026
N9 N 0.61382 0.32157 0.35779
N10 N 0.69956 0.30857 0.79561
H*11 H 0.67798 0.20185 0.85409
H*12 H 0.58625 0.41972 0.31197
H*13 H 0.60510 0.22451 0.29003
H*14 H 0.65918 0.39661 0.87599
C1+ C 0.09035 0.67340 0.08637
N'2+ N 0.03035 0.61253 0.23862
N'3+ N 0.04356 0.45760 0.21474
N'4+ N 0.10946 0.42801 0.05304
N'5+ N 0.14009 0.56326 -0.03064
N6+ N 0.10038 0.84035 0.05197
O7+ O 0.05129 0.93230 0.16843
O8+ O 0.15765 0.88455 -0.09254

#END

data_T_DAGH_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 15.641
_cell_length_b 6.599
_cell_length_c 16.899
_cell_angle_alpha 90.00
_cell_angle_beta 94.58
_cell_angle_gamma 90.00
_cell_volume 1738.66
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.50209 0.57458 -0.37344
N2 N 0.42745 0.66201 -0.39816
H*3 H 0.42905 0.80813 -0.41703
N4 N 0.57516 0.68240 -0.37460
H*5 H 0.63202 0.61745 -0.35598
N6 N 0.50389 0.38336 -0.34804
H*7 H 0.44737 0.30807 -0.34821
H*8 H 0.55925 0.31379 -0.32909
N9 N 0.57088 0.88298 -0.40165
N10 N 0.35168 0.54915 -0.39682
H*11 H 0.32263 0.53767 -0.45276
H*12 H 0.59366 0.97916 -0.35781
H*13 H 0.60500 0.89908 -0.45012
H*14 H 0.31131 0.61756 -0.36067
C1+ C 0.20096 0.39401 0.33228
N'2+ N 0.12614 0.36433 0.28907
N'3+ N 0.14950 0.33617 0.21605
N'4+ N 0.23561 0.34890 0.21621
N'5+ N 0.26954 0.38553 0.28935
N6+ N 0.20704 0.43129 0.41637
O7+ O 0.14003 0.43621 0.45052
O8+ O 0.27902 0.45676 0.45079

#END

S12. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidinium 5-nitrotetrazolate (ionic form).
data_T_TAGH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.286
_cell_length_b                 12.670
_cell_length_c                 8.431
_cell_angle_alpha               90.00
_cell_angle_beta               135.33
_cell_angle_gamma                90.00
_cell_volume                   922.647
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.24584 0.50484 0.26316
N2 N -0.24268 0.60506 0.31736
H*3 H -0.24715 0.61757 0.43173
N4 N -0.24022 0.48395 0.11321
H*5 H -0.23362 0.54627 0.04443
N6 N -0.25462 0.42552 0.35891
H*7 H -0.25675 0.35067 0.31332
N8 N -0.24370 0.37854 0.05942
N9 N -0.23347 0.68654 0.21493
H*10 H -0.13541 0.72955 0.33454
H*11 H -0.33786 0.36603 -0.10839
H*12 H -0.14543 0.36124 0.09975
H*13 H -0.32784 0.73434 0.12640
N14 N -0.26035 0.44944 0.51513
H*15 H -0.36046 0.42134 0.45925
H*16 H -0.16803 0.41655 0.66739
C1+ C 0.22944 0.35506 0.23681
N'2+ N 0.16056 0.30523 0.28707
N'3+ N 0.01066 0.31670 0.10136
N'4+ N -0.00824 0.37172 -0.05388
N'5+ N 0.12908 0.39685 0.02855
N6+ N 0.39469 0.36292 0.39108
O7+ O 0.47732 0.32172 0.57927
O8+ O 0.44681 0.41052 0.32871

#END

data_T_TAGH_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P n a 21'
_symmetry_Int_Tables_number      33
loop_
_symmetry_equiv_pos_site_id
_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
```

```
_cell_length_a                 12.568
_cell_length_b                 8.460
_cell_length_c                 8.667
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   921.521
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.49529 0.01235 0.26631
N2 N 0.39410 0.06248 0.26604
H*3 H 0.38124 0.18110 0.26730
N4 N 0.51666 -0.14289 0.26469
H*5 H 0.45394 -0.21874 0.26329
N6 N 0.57510 0.11746 0.26820
H*7 H 0.65069 0.07468 0.26834
N8 N 0.62310 -0.19226 0.26502
N9 N 0.31211 -0.04975 0.26405
H*10 H 0.26668 -0.03529 0.16779
H*11 H 0.63787 -0.25902 0.36041
H*12 H 0.63864 -0.25669 0.16836
H*13 H 0.26591 -0.03762 0.35985
N14 N 0.55066 0.27906 0.26986
H*15 H 0.58094 0.33019 0.36675
H*16 H 0.58171 0.33252 0.17470
C1+ C 0.14569 -0.00768 0.75272
N'2+ N 0.19042 -0.12986 0.67796
N'3+ N 0.17384 -0.09600 0.53033
N'4+ N 0.12086 0.04218 0.51844
N'5+ N 0.10220 0.10024 0.65815
N6+ N 0.14450 0.00624 0.91805
O7+ O 0.18676 -0.09959 0.99505
O8+ O 0.10125 0.12343 0.97586

#END

data_T_TAGH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.607
```

```
_cell_length_b                 8.530
_cell_length_c                 12.638
_cell_angle_alpha               90.00
_cell_angle_beta                83.71
_cell_angle_gamma                 90.00
_cell_volume                   922.267
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24100 0.49101 -0.00718
N2 N 0.23947 0.43865 -0.10708
H*3 H 0.24285 0.32074 -0.11874
N4 N 0.23672 0.64544 0.01259
H*5 H 0.23237 0.71896 -0.05031
N6 N 0.24681 0.38893 0.07295
H*7 H 0.24778 0.43332 0.14751
N8 N 0.23844 0.69718 0.11769
N9 N 0.23337 0.54774 -0.18942
H*10 H 0.13515 0.53024 -0.22607
H*11 H 0.33404 0.76569 0.12345
H*12 H 0.13960 0.75949 0.14080
H*13 H 0.32960 0.53645 -0.24342
N14 N 0.25120 0.22812 0.05019
H*15 H 0.35103 0.18020 0.07240
H*16 H 0.15658 0.17399 0.08976
C1+ C 0.24266 0.49176 0.35730
N'2+ N 0.17631 0.37107 0.31085
N'3+ N 0.02615 0.41004 0.31854
N'4+ N 0.00464 0.54969 0.36811
N'5+ N 0.14048 0.60363 0.39340
N6+ N 0.40722 0.50037 0.36742
O7+ O 0.49167 0.39118 0.33155
O8+ O 0.45695 0.61658 0.41155

#END

data_T_TAGH_4
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 12.685
_cell_length_b 8.554
_cell_length_c 17.151
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1861.01
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24645 0.73686 0.34840
N2 N 0.15030 0.72680 0.31633
H*3 H 0.14595 0.71627 0.25739
N4 N 0.25663 0.75091 0.42589
H*5 H 0.18954 0.75350 0.45828
N6 N 0.33242 0.73286 0.30298
H*7 H 0.40387 0.74081 0.32954
N8 N 0.35799 0.76122 0.45797
N9 N 0.06169 0.73126 0.36508
H*10 H 0.01953 0.63059 0.35938
H*11 H 0.36629 0.86440 0.48694
H*12 H 0.37035 0.67062 0.49539
H*13 H 0.01546 0.82437 0.35093
N14 N 0.31967 0.71810 0.22216
H*15 H 0.35150 0.81247 0.19466
H*16 H 0.35557 0.61869 0.20311
C1+ C 0.09892 0.71693 0.10208
N'2+ N 0.07125 0.63441 0.16549
N'3+ N 0.08429 0.48704 0.14319
N'4+ N 0.11866 0.48284 0.06877
N'5+ N 0.12848 0.62742 0.04156
N6+ N 0.09706 0.88490 0.09926
O7+ O 0.06857 0.95677 0.15817
O8+ O 0.12404 0.95000 0.03805

#END

data_T_TAGH_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.602
_cell_length_b                 12.648
_cell_length_c                 8.552
_cell_angle_alpha               90.00
_cell_angle_beta                93.35
_cell_angle_gamma                 90.00
_cell_volume                   928.851
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.30171 0.74695 0.25263
N2 N -0.36546 0.65028 0.25491
H*3 H -0.48308 0.64556 0.25952
N4 N -0.14712 0.75763 0.24659
H*5 H -0.08233 0.69051 0.24390
N6 N -0.39255 0.83293 0.25639
H*7 H -0.33973 0.90478 0.25448
N8 N -0.08334 0.85953 0.24432
N9 N -0.26799 0.56167 0.25089
H*10 H -0.29711 0.51737 0.15414
H*11 H -0.00771 0.87000 0.33916
H*12 H -0.02654 0.87020 0.14432
H*13 H -0.27828 0.51717 0.34898
N14 N -0.55379 0.81965 0.26268
H*15 H -0.59089 0.85338 0.36200
H*16 H -0.60973 0.85358 0.16716
C1+ C 0.79593 0.09990 0.26102
N'2+ N 0.91627 0.12814 0.35934
N'3+ N 0.86163 0.11491 0.50003
N'4+ N 0.71334 0.07989 0.48505
N'5+ N 0.66933 0.06982 0.33439
N6+ N 0.80204 0.10172 0.09339
O7+ O 0.92420 0.13072 0.03713
O8+ O 0.68487 0.07419 0.01295

#END
```

S13. Optimized crystal structure coordinates for 5 polymorphs of Ammonium 5-(trinitromethyl)tetrazolate (ionic form).

```
data_FTNM_NH4_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 11.792
_cell_length_b                 13.094
_cell_length_c                 13.984
_cell_angle_alpha               90.00
_cell_angle_beta               124.68
_cell_angle_gamma                90.00
_cell_volume                  1775.6
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.13678 0.01249 0.42089
H*2 H 0.14782 0.07921 0.38822
H*3 H 0.18855 -0.04532 0.41133
H*4 H 0.17681 0.02187 0.50758
H*5 H 0.03394 -0.00580 0.37643
C1+ C -0.18439 0.36539 0.30204
N'2+ N -0.37063 0.44234 0.18548
N'3+ N -0.30279 0.43166 0.13540
N'4+ N -0.18448 0.38262 0.20716
N'5+ N -0.29814 0.40100 0.29133
C6+ C -0.06997 0.31221 0.40389
N7+ N -0.10999 0.27021 0.48414
O8+ O -0.11972 0.17816 0.49012
O9+ O -0.12903 0.33580 0.53509
N10+ N -0.01659 0.22355 0.36477
O11+ O -0.10186 0.16012 0.30177
O12+ O 0.10423 0.22610 0.39835
N13+ N 0.06284 0.37964 0.48867
O14+ O 0.07374 0.45861 0.44951
O15+ O 0.14304 0.34541 0.58637

#END

data_FTNM_NH4_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.604
_cell_length_b 6.954
_cell_length_c 12.286
_cell_angle_alpha 90.00
_cell_angle_beta 68.67
_cell_angle_gamma 90.00
_cell_volume 843.914
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.32056 -0.29474 0.50180
H*2 H 0.21947 -0.29507 0.55336
H*3 H 0.37745 -0.30600 0.55370
H*4 H 0.34120 -0.40923 0.44508
H*5 H 0.34412 -0.16866 0.45506
C1+ C 0.68416 -0.26665 0.14596
N'2+ N 0.50878 -0.24455 0.10484
N'3+ N 0.53881 -0.43079 0.10757
N'4+ N 0.64931 -0.44924 0.13403
N'5+ N 0.59917 -0.13669 0.12890
C6+ C 0.80295 -0.22201 0.17548
N7+ N 0.79873 -0.01565 0.22331
O8+ O 0.78173 0.00596 0.32608
O9+ O 0.81288 0.10973 0.15087
N10+ N 0.81622 -0.37038 0.26600
O11+ O 0.71927 -0.38180 0.35656
O12+ O 0.92043 -0.46434 0.23800
N13+ N 0.94464 -0.23093 0.06997
O14+ O 0.94786 -0.31854 -0.01616
O15+ O 1.03857 -0.14873 0.08535

#END

data_FTNM_NH4_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 9.471
_cell_length_b 8.226
_cell_length_c 10.934
_cell_angle_alpha 90.00

```
_cell_angle_beta                 83.46
_cell_angle_gamma                90.00
_cell_volume                    846.308
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.71319 0.62021 0.54367
H*2 H -0.81951 0.62968 0.53377
H*3 H -0.69412 0.51058 0.58379
H*4 H -0.65477 0.62733 0.45866
H*5 H -0.68437 0.71325 0.59846
C1+ C -0.36194 0.65503 0.19281
N'2+ N -0.53832 0.65810 0.32828
N'3+ N -0.57637 0.72615 0.22594
N'4+ N -0.46673 0.72515 0.13817
N'5+ N -0.40279 0.61164 0.31015
C6+ C -0.22010 0.63024 0.12674
N7+ N -0.13305 0.50203 0.18924
O8+ O -0.10828 0.37187 0.13814
O9+ O -0.09687 0.54523 0.28732
N10+ N -0.23207 0.57986 -0.00928
O11+ O -0.30137 0.45855 -0.02248
O12+ O -0.17394 0.66695 -0.09029
N13+ N -0.11946 0.78536 0.11616
O14+ O -0.17644 0.91634 0.13384
O15+ O 0.00729 0.75864 0.09047

#END

data_FTNM_NH4_4
_symmetry_cell_setting           monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  10.421
_cell_length_b                  7.963
_cell_length_c                  10.653
_cell_angle_alpha                90.00
_cell_angle_beta                 108.20
_cell_angle_gamma                90.00
_cell_volume                    839.786
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.31026 0.40183 -0.59290
H*2 H 0.20799 0.37964 -0.62304
H*3 H 0.35379 0.33560 -0.65187
H*4 H 0.32752 0.52798 -0.60030
H*5 H 0.35174 0.36410 -0.49639
C1+ C -0.33979 0.17863 0.73842
N'2+ N -0.52814 0.22046 0.76658
N'3+ N -0.53028 0.28957 0.65156
N'4+ N -0.41227 0.26426 0.63076
N'5+ N -0.40857 0.14898 0.82406
C6+ C -0.20090 0.12505 0.75523
N7+ N -0.15358 -0.01635 0.85876
O8+ O -0.13657 -0.15672 0.82133
O9+ O -0.13782 0.02810 0.97175
N10+ N -0.18730 0.06669 0.62012
O11+ O -0.26203 -0.04628 0.56581
O12+ O -0.10562 0.14041 0.57926
N13+ N -0.08834 0.26567 0.80574
O14+ O -0.12653 0.41011 0.79397
O15+ O 0.02762 0.21532 0.85178

#END

data_FTNM_NH4_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 11.300
_cell_length_b                 8.817
_cell_length_c                 9.167
_cell_angle_alpha               90.00
_cell_angle_beta               102.48
_cell_angle_gamma                90.00
_cell_volume                   891.747
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.49712 -0.36619 -0.21678
```

H*2 H 0.43027 -0.38249 -0.15809
H*3 H 0.54740 -0.27227 -0.17600
H*4 H 0.55251 -0.45987 -0.20516
H*5 H 0.45830 -0.35013 -0.32787
C1+ C 0.23423 0.64539 -0.86988
N'2+ N 0.32931 0.63777 -1.04320
N'3+ N 0.22639 0.71482 -1.09144
N'4+ N 0.16444 0.72214 -0.98351
N'5+ N 0.33694 0.59224 -0.90290
C6+ C 0.19817 0.62606 -0.72676
N7+ N 0.30588 0.58221 -0.59893
O8+ O 0.34289 0.67447 -0.50076
O9+ O 0.34485 0.45513 -0.60968
N10+ N 0.13718 0.77396 -0.68510
O11+ O 0.19839 0.88781 -0.67676
O12+ O 0.03348 0.76400 -0.66732
N13+ N 0.10135 0.49639 -0.72234
O14+ O 0.04339 0.45208 -0.84152
O15+ O 0.09354 0.45300 -0.59825

#END

S14. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylammonium 5-(trinitromethyl)tetrazolate (ionic form).

data_FTNM_NH3OH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 12.507
_cell_length_b 10.099
_cell_length_c 7.750
_cell_angle_alpha 90.00
_cell_angle_beta 105.17
_cell_angle_gamma 90.00
_cell_volume 944.778
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.58569 0.38414 0.24910
H*2 H 0.59915 0.38328 0.12347
H*3 H 0.50495 0.41297 0.23818
H*4 H 0.60013 0.29036 0.30340

O5 O 0.66223 0.47674 0.34574
H*6 H 0.65216 0.48060 0.46643
C1+ C 0.26896 0.08970 0.78959
N'2+ N 0.15891 0.08179 0.95318
N'3+ N 0.11504 0.01306 0.80402
N'4+ N 0.18334 0.01580 0.69803
N'5+ N 0.25666 0.13164 0.94806
C6+ C 0.36419 0.11776 0.71841
N7+ N 0.46687 0.16339 0.86488
O8+ O 0.54654 0.08970 0.90782
O9+ O 0.45749 0.27245 0.92563
N10+ N 0.39360 -0.00674 0.62074
O11+ O 0.41423 -0.10630 0.71064
O12+ O 0.39145 0.00513 0.46314
N13+ N 0.34684 0.23267 0.57368
O14+ O 0.25214 0.26348 0.50148
O15+ O 0.43112 0.27974 0.54734

#END

data_FTNM_NH3OH_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 13.048
_cell_length_b 8.139
_cell_length_c 9.219
_cell_angle_alpha 90.00
_cell_angle_beta 101.85
_cell_angle_gamma 90.00
_cell_volume 958.172
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.32453 0.41138 0.15012
H*2 H 0.34162 0.28989 0.13429
H*3 H 0.25474 0.44094 0.07956
H*4 H 0.31901 0.42782 0.25935
O5 O 0.40917 0.49911 0.11550
H*6 H 0.39597 0.61562 0.12916
C1+ C -0.01210 0.59981 0.23687
N'2+ N -0.11499 0.41123 0.14382

N'3+ N -0.14794 0.55205 0.07517
N'4+ N -0.08382 0.67378 0.13143
N'5+ N -0.02888 0.43751 0.24704
C6+ C 0.07432 0.69216 0.32742
N7+ N 0.16498 0.57969 0.40339
O8+ O 0.24768 0.58493 0.36174
O9+ O 0.14385 0.49326 0.50071
N10+ N 0.11608 0.82368 0.23083
O11+ O 0.14613 0.77109 0.12383
O12+ O 0.11333 0.96713 0.26845
N13+ N 0.04585 0.79332 0.46118
O14+ O -0.04607 0.82065 0.45569
O15+ O 0.11974 0.83545 0.55808

#END

data_FTNM_NH3OH_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 19.233
_cell_length_b 9.306
_cell_length_c 10.903
_cell_angle_alpha 90.00
_cell_angle_beta 105.35
_cell_angle_gamma 90.00
_cell_volume 1881.83
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.32540 0.21879 -0.17041
H*2 H 0.34223 0.26602 -0.24312
H*3 H 0.36875 0.16730 -0.11008
H*4 H 0.30524 0.29750 -0.12251
O5 O 0.27161 0.12111 -0.23160
H*6 H 0.25410 0.07372 -0.16561
C1+ C -0.13707 -0.15042 0.51562
N'2+ N -0.20222 -0.00742 0.58526

N'3+ N -0.18879 0.05055 0.48168
N'4+ N -0.14784 -0.03816 0.43506
N'5+ N -0.17014 -0.13506 0.60924
C6+ C -0.09374 -0.27448 0.49822
N7+ N -0.10812 -0.40835 0.57168
O8+ O -0.13945 -0.51041 0.51174
O9+ O -0.08609 -0.39799 0.68659
N10+ N -0.10817 -0.31059 0.35389
O11+ O -0.17043 -0.33559 0.29862
O12+ O -0.05668 -0.30811 0.30826
N13+ N -0.00883 -0.25403 0.54640
O14+ O 0.01321 -0.13176 0.56233
O15+ O 0.02695 -0.36418 0.56272

#END

data_FTNM_NH3OH_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 12.509
_cell_length_b 9.859
_cell_length_c 7.867
_cell_angle_alpha 90.00
_cell_angle_beta 109.24
_cell_angle_gamma 90.00
_cell_volume 916.018
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.42317 -0.12245 0.15924
H*2 H 0.39869 -0.09579 0.02517
H*3 H 0.42323 -0.22693 0.16897
H*4 H 0.50301 -0.08375 0.22392
O5 O 0.34130 -0.06320 0.22274
H*6 H 0.36149 -0.08618 0.35022
C1+ C 0.78105 0.10232 0.30517
N'2+ N 0.67660 0.07680 0.46453
N'3+ N 0.62646 0.01789 0.30496
N'4+ N 0.69110 0.03190 0.20131
N'5+ N 0.77493 0.13127 0.46885
C6+ C 0.87422 0.14008 0.24046

```
N7+ N 0.98318 0.17766 0.39555
O8+ O 1.06432 0.10165 0.42997
O9+ O 0.97677 0.28330 0.47127
N10+ N 0.89925 0.02250 0.12623
O11+ O 0.92268 -0.08578 0.20240
O12+ O 0.89125 0.04780 -0.02938
N13+ N 0.85213 0.26874 0.11183
O14+ O 0.75450 0.30302 0.04180
O15+ O 0.93612 0.32171 0.09426

#END

data_FTNM_NH3OH_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 10.323
_cell_length_b                 9.490
_cell_length_c                 9.696
_cell_angle_alpha               90.00
_cell_angle_beta               105.20
_cell_angle_gamma                90.00
_cell_volume                   916.641
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.25994 0.46429 0.84351
H*2 H 0.17080 0.51524 0.79803
H*3 H 0.29402 0.41731 0.76353
H*4 H 0.32864 0.53705 0.89871
O5 O 0.22707 0.36399 0.93556
H*6 H 0.30936 0.31303 0.98113
C1+ C 0.59858 0.11691 0.21898
N'2+ N 0.44926 0.24337 0.08689
N'3+ N 0.56805 0.30625 0.10186
N'4+ N 0.66480 0.22801 0.18461
N'5+ N 0.46532 0.12289 0.15995
C6+ C 0.66940 0.00337 0.31084
N7+ N 0.58477 -0.13268 0.29743
O8+ O 0.61873 -0.23520 0.23984
O9+ O 0.48860 -0.12343 0.34721
N10+ N 0.80554 -0.02865 0.27568
```

O11+ O 0.79759 -0.06106 0.15283
O12+ O 0.90781 -0.01608 0.37246
N13+ N 0.70917 0.03530 0.47753
O14+ O 0.70988 0.15777 0.51268
O15+ O 0.73622 -0.06718 0.55601

#END

S15. Optimized crystal structure coordinates for 5 polymorphs of Hydrazinium 5-(trinitromethyl)tetrazolate (ionic form).

data_FTNM_N2H5_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.492
_cell_length_b 13.192
_cell_length_c 7.088
_cell_angle_alpha 90.00
_cell_angle_beta 71.21
_cell_angle_gamma 90.00
_cell_volume 928.769
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.87765 -0.13410 0.14054
H*2 H 0.92606 -0.10595 0.00036
H*3 H 0.94023 -0.18802 0.16814
N4 N 0.75561 -0.18408 0.13678
H*5 H 0.70895 -0.21279 0.27583
H*6 H 0.69469 -0.13026 0.10709
H*7 H 0.86544 -0.07611 0.24274
C1+ C 0.18159 0.59535 -0.02408
N'2+ N 0.02646 0.61370 0.24880
N'3+ N 0.02937 0.69571 0.13668
N'4+ N 0.12643 0.68596 -0.03783
N'5+ N 0.12186 0.54857 0.15084
C6+ C 0.29436 0.55498 -0.18791
N7+ N 0.31171 0.43938 -0.17092
O8+ O 0.28567 0.38376 -0.29073
O9+ O 0.35074 0.41436 -0.03381
N10+ N 0.27550 0.58074 -0.39215
O11+ O 0.17220 0.55017 -0.41390

O12+ O 0.36364 0.63052 -0.51043
N13+ N 0.43853 0.59914 -0.20487
O14+ O 0.44086 0.67805 -0.11886
O15+ O 0.53493 0.54945 -0.30453

#END

data_FTNM_N2H5_2
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 8.062
_cell_length_b 7.019
_cell_length_c 10.592
_cell_angle_alpha 118.16
_cell_angle_beta 111.48
_cell_angle_gamma 76.03
_cell_volume 490.002
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.36831 0.30346 0.64583
H*2 H -0.48450 0.27210 0.55813
H*3 H -0.28613 0.16186 0.62244
N4 N -0.41138 0.35407 0.78018
H*5 H -0.29507 0.38260 0.86636
H*6 H -0.49458 0.49346 0.80168
H*7 H -0.30791 0.42078 0.64946
C1+ C -0.04745 -0.15017 0.71636
N'2+ N -0.23501 -0.36575 0.65235
N'3+ N -0.30577 -0.24234 0.57727
N'4+ N -0.18936 -0.10467 0.61509
N'5+ N -0.07104 -0.31119 0.74154
C6+ C 0.11351 -0.03252 0.78768
N7+ N 0.27813 -0.15490 0.85828
O8+ O 0.39928 -0.23244 0.80100
O9+ O 0.26986 -0.16265 0.96805
N10+ N 0.15472 0.01277 0.67183
O11+ O 0.17519 -0.14599 0.56077
O12+ O 0.15959 0.20173 0.70040
N13+ N 0.10231 0.19940 0.92237
O14+ O -0.04584 0.28254 0.93050
O15+ O 0.24508 0.27423 1.00602

```
#END

data_FTNM_N2H5_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 11.868
_cell_length_b                 11.799
_cell_length_c                 7.174
_cell_angle_alpha               90.00
_cell_angle_beta                69.31
_cell_angle_gamma               90.00
_cell_volume                   939.789
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.86478 0.48907 0.30016
H*2 H 0.84477 0.54195 0.20215
H*3 H 0.95473 0.46936 0.23629
N4 N 0.79619 0.38561 0.31735
H*5 H 0.81757 0.33309 0.41312
H*6 H 0.70698 0.40609 0.37878
H*7 H 0.85122 0.53260 0.43120
C1+ C 0.28054 -0.62957 1.04160
N'2+ N 0.16890 -0.57700 1.32725
N'3+ N 0.10913 -0.56277 1.20210
N'4+ N 0.17757 -0.59597 1.01985
N'5+ N 0.27799 -0.61933 1.22983
C6+ C 0.38195 -0.67302 0.87289
N7+ N 0.47210 -0.74127 0.93988
O8+ O 0.47901 -0.84337 0.91307
O9+ O 0.52918 -0.68411 1.01637
N10+ N 0.33493 -0.74785 0.73645
O11+ O 0.27298 -0.82794 0.81739
O12+ O 0.36190 -0.71902 0.56271
N13+ N 0.46383 -0.57976 0.72771
O14+ O 0.42074 -0.48606 0.73601
O15+ O 0.56350 -0.61116 0.61925

#END

data_FTNM_N2H5_4
```

```
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 19.925
_cell_length_b                 13.166
_cell_length_c                 7.059
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1851.81
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.06052 0.13412 0.07967
H*2 H -0.02704 0.18680 0.13116
H*3 H -0.03958 0.10449 -0.04151
N4 N -0.12155 0.18688 0.02749
H*5 H -0.15423 0.13425 -0.02544
H*6 H -0.14162 0.21703 0.14821
H*7 H -0.06566 0.07658 0.17806
C1+ C 0.09123 0.09329 0.56275
N'2+ N 0.01107 0.11188 0.75334
N'3+ N 0.01628 0.19610 0.64856
N'4+ N 0.06654 0.18628 0.52566
N'5+ N 0.05795 0.04515 0.70219
C6+ C 0.14830 0.05203 0.45682
N7+ N 0.15386 -0.06463 0.47479
O8+ O 0.14188 -0.11689 0.33647
O9+ O 0.17006 -0.09390 0.63158
N10+ N 0.14313 0.08265 0.24377
O11+ O 0.09223 0.05632 0.16361
O12+ O 0.18943 0.13158 0.17674
N13+ N 0.22018 0.09121 0.52138
O14+ O 0.22166 0.16835 0.61465
O15+ O 0.26792 0.03993 0.47020

#END
```

```
data_FTNM_N2H5_5
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                  10.462
_cell_length_b                  5.976
_cell_length_c                  7.535
_cell_angle_alpha                100.58
_cell_angle_beta                 85.43
_cell_angle_gamma                80.17
_cell_volume                    453.28
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.70628 0.37459 -0.07941
H*2 H 0.66142 0.45226 0.04883
H*3 H 0.79708 0.28790 -0.06347
N4 N 0.72401 0.55530 -0.17824
H*5 H 0.76991 0.47687 -0.30464
H*6 H 0.63347 0.64216 -0.19171
H*7 H 0.65319 0.25530 -0.13730
C1+ C 0.33241 0.09353 -0.25267
N'2+ N 0.52427 0.10987 -0.19457
N'3+ N 0.50973 -0.11121 -0.21763
N'4+ N 0.38908 -0.12701 -0.25558
N'5+ N 0.41340 0.24411 -0.21602
C6+ C 0.19640 0.15375 -0.28814
N7+ N 0.16494 0.39453 -0.33908
O8+ O 0.14428 0.40520 -0.49441
O9+ O 0.16433 0.55587 -0.21432
N10+ N 0.16472 -0.03513 -0.44190
O11+ O 0.23320 -0.06958 -0.58537
O12+ O 0.07656 -0.13477 -0.40505
N13+ N 0.08925 0.16981 -0.12221
O14+ O 0.12425 0.07652 0.00002
O15+ O -0.01982 0.27476 -0.13303

#END
```

S16. Optimized crystal structure coordinates for 5 polymorphs of Guanidinium 5-(trinitromethyl)tetrazolate (ionic form).

```
data_FTNM_GH_1
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
```

```
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 11.512
_cell_length_b                 12.188
_cell_length_c                 14.996
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   2104.06
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.22562 0.02309 0.50387
N2 N 0.26146 0.11378 0.54586
H*3 H 0.33652 0.15133 0.52886
H*4 H 0.21452 0.14741 0.59581
N5 N 0.28951 -0.01963 0.43798
H*6 H 0.26404 -0.08809 0.40538
H*7 H 0.36513 0.01530 0.41886
N8 N 0.12589 -0.02488 0.52777
H*9 H 0.07629 0.00604 0.57738
H*10 H 0.09721 -0.09345 0.49693
C1+ C 0.05835 0.30353 0.65573
N'2+ N -0.05734 0.29966 0.54727
N'3+ N -0.01850 0.19783 0.56172
N'4+ N 0.05466 0.19768 0.63047
N'5+ N -0.01017 0.36864 0.60590
C6+ C 0.13042 0.33962 0.73074
N7+ N 0.09299 0.45275 0.76728
O8+ O 0.04788 0.45749 0.84066
O9+ O 0.11267 0.52881 0.71708
N10+ N 0.12722 0.25253 0.80698
O11+ O 0.03160 0.23089 0.83587
O12+ O 0.21955 0.21219 0.82993
N13+ N 0.26461 0.35536 0.70948
O14+ O 0.30125 0.31108 0.64291
O15+ O 0.31942 0.41074 0.76274

#END
```

```
data_FTNM_GH_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.882
_cell_length_b                 10.765
_cell_length_c                 11.019
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1053.58
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.48767 0.72245 0.40701
N2 N 0.48455 0.67152 0.29634
H*3 H 0.53061 0.71513 0.22411
H*4 H 0.43604 0.58794 0.28171
N5 N 0.55264 0.83320 0.42372
H*6 H 0.55625 0.87335 0.50657
H*7 H 0.60004 0.87998 0.35399
N8 N 0.42582 0.66263 0.50097
H*9 H 0.37616 0.57887 0.49035
H*10 H 0.42693 0.69943 0.58533
C1+ C -0.05436 0.89738 0.15828
N'2+ N -0.27324 0.90889 0.23010
N'3+ N -0.26601 0.98089 0.13142
N'4+ N -0.12858 0.97494 0.08356
N'5+ N -0.14064 0.85456 0.24951
C6+ C 0.10388 0.86521 0.13767
N7+ N 0.15135 0.74618 0.20604
O8+ O 0.17841 0.65269 0.14769
O9+ O 0.15672 0.75793 0.31567
N10+ N 0.13461 0.84969 -0.00093
O11+ O 0.05795 0.77276 -0.05223
O12+ O 0.22986 0.91683 -0.04645
N13+ N 0.22331 0.96562 0.18128
O14+ O 0.17692 1.06996 0.19814
O15+ O 0.35236 0.92856 0.19355

#END
```

```
data_FTNM_GH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 18.381
_cell_length_b                 8.151
_cell_length_c                 7.845
_cell_angle_alpha               90.00
_cell_angle_beta                61.71
_cell_angle_gamma                90.00
_cell_volume                   1034.98
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.49876 -0.25657 0.92423
N2 N 0.43232 -0.15910 0.99414
H*3 H 0.40740 -0.11374 1.13010
H*4 H 0.40511 -0.12796 0.91304
N5 N 0.53351 -0.29577 1.03483
H*6 H 0.58374 -0.36921 0.98487
H*7 H 0.51057 -0.25308 1.17159
N8 N 0.53044 -0.31484 0.74373
H*9 H 0.50515 -0.28676 0.65772
H*10 H 0.58060 -0.38866 0.68806
C1+ C 0.14898 0.48377 0.40359
N'2+ N 0.05381 0.33433 0.60504
N'3+ N 0.05360 0.32347 0.43524
N'4+ N 0.11363 0.41643 0.30432
N'5+ N 0.11368 0.43515 0.58960
C6+ C 0.21902 0.59679 0.31110
N7+ N 0.26710 0.61496 0.42681
O8+ O 0.33643 0.55759 0.35968
O9+ O 0.22938 0.68708 0.57976
N10+ N 0.27860 0.53879 0.10065
O11+ O 0.30610 0.40137 0.08622
O12+ O 0.29134 0.63369 -0.03095
N13+ N 0.19634 0.78045 0.28710
O14+ O 0.12892 0.80310 0.29940
O15+ O 0.24941 0.88317 0.25738

#END
```

```
data_FTNM_GH_4
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 8.140
_cell_length_b                 7.543
_cell_length_c                 8.526
_cell_angle_alpha               85.70
_cell_angle_beta                95.08
_cell_angle_gamma               93.36
_cell_volume                   519.26
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.44172 0.25922 -0.12126
N2 N 0.60352 0.29546 -0.08946
H*3 H 0.67964 0.32055 -0.17682
H*4 H 0.65440 0.29881 0.02286
N5 N 0.37775 0.25568 -0.27105
H*6 H 0.25584 0.22858 -0.29769
H*7 H 0.44944 0.27999 -0.36196
N8 N 0.34389 0.22652 -0.00327
H*9 H 0.38968 0.22852 0.11073
H*10 H 0.22132 0.19886 -0.02467
C1+ C 0.77250 0.26547 -0.65585
N'2+ N 0.56552 0.27403 -0.52604
N'3+ N 0.51256 0.25188 -0.67661
N'4+ N 0.64126 0.24507 -0.76166
N'5+ N 0.73001 0.28307 -0.50907
C6+ C 0.94177 0.26608 -0.70187
N7+ N 1.06900 0.23020 -0.55911
O8+ O 1.13692 0.08953 -0.54531
O9+ O 1.08911 0.35042 -0.47090
N10+ N 0.95351 0.12592 -0.82553
O11+ O 0.91177 -0.02594 -0.78375
O12+ O 1.00000 0.17998 -0.95360
N13+ N 1.01065 0.44802 -0.78417
O14+ O 0.90951 0.55264 -0.83794
O15+ O 1.16051 0.46608 -0.78650

#END

data_FTNM_GH_5
```

```
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 10.193
_cell_length_b                 11.806
_cell_length_c                 9.049
_cell_angle_alpha               90.00
_cell_angle_beta               101.75
_cell_angle_gamma                90.00
_cell_volume                   1066.13
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.64943 -0.32157 0.76288
N2 N 0.58447 -0.32305 0.87723
H*3 H 0.51584 -0.38343 0.88467
H*4 H 0.60211 -0.26383 0.95953
N5 N 0.62406 -0.40102 0.65551
H*6 H 0.67200 -0.40148 0.56814
H*7 H 0.55620 -0.46293 0.65861
N8 N 0.73976 -0.24064 0.75590
H*9 H 0.76045 -0.17980 0.83583
H*10 H 0.78997 -0.23795 0.67050
C1+ C 0.28189 -0.09255 0.27033
N'2+ N 0.10056 -0.01341 0.28656
N'3+ N 0.13675 0.02279 0.16067
N'4+ N 0.25117 -0.02646 0.14702
N'5+ N 0.19066 -0.08676 0.35862
C6+ C 0.40305 -0.16265 0.29941
N7+ N 0.39635 -0.25823 0.41428
O8+ O 0.38661 -0.35589 0.36997
O9+ O 0.40119 -0.22518 0.54250
N10+ N 0.42805 -0.21416 0.14875
O11+ O 0.33747 -0.27110 0.07857
O12+ O 0.53409 -0.19160 0.11262
N13+ N 0.53833 -0.09829 0.36947
O14+ O 0.53742 0.00386 0.35742
O15+ O 0.63209 -0.15797 0.42915

#END
```

S17. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidinium 5-(trinitromethyl)tetrazolate (ionic form).

```
data_FTNM_AGH_1
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 6.914
_cell_length_b                 6.884
_cell_length_c                 13.927
_cell_angle_alpha               64.40
_cell_angle_beta               109.03
_cell_angle_gamma               89.69
_cell_volume                   556.743
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.75887 0.17486 0.15507
N2 N 0.63286 0.21192 0.05047
H*3 H 0.48032 0.20295 0.03255
H*4 H 0.68711 0.24994 -0.01350
N5 N 0.68042 0.12462 0.23800
H*6 H 0.52734 0.11535 0.22057
N7 N 0.95959 0.18671 0.17856
H*8 H 1.02406 0.22392 0.11865
H*9 H 1.04805 0.15715 0.25914
N10 N 0.81281 0.08608 0.34710
H*11 H 0.76456 0.19639 0.36865
H*12 H 0.81732 -0.06905 0.40573
C1+ C 0.06156 0.64659 0.18239
N'2+ N -0.22047 0.74717 0.04244
N'3+ N -0.06587 0.72704 0.00779
N'4+ N 0.11494 0.66233 0.09497
N'5+ N -0.14456 0.69713 0.15292
C6+ C 0.21804 0.57892 0.29652
N7+ N 0.12327 0.50050 0.39053
O8+ O 0.16190 0.30714 0.45880
O9+ O 0.01466 0.64513 0.38668
N10+ N 0.39093 0.39505 0.32459
O11+ O 0.33159 0.23240 0.32058
O12+ O 0.56886 0.43069 0.34586
N13+ N 0.33964 0.76369 0.31367
O14+ O 0.33394 0.92278 0.22791
O15+ O 0.42944 0.72828 0.41254
```

```
#END

data_FTNM_AGH_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 25.437
_cell_length_b                 6.890
_cell_length_c                 6.896
_cell_angle_alpha               90.00
_cell_angle_beta                68.63
_cell_angle_gamma                90.00
_cell_volume                   1125.5
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.57318 0.19017 0.23659
N2 N 0.52144 0.24615 0.36118
H*3 H 0.51223 0.27222 0.51422
H*4 H 0.49015 0.26385 0.30531
N5 N 0.61372 0.16825 0.31718
H*6 H 0.60474 0.19420 0.47078
N7 N 0.58526 0.15590 0.03520
H*8 H 0.55599 0.17076 -0.03087
H*9 H 0.62510 0.11386 -0.05211
N10 N 0.66769 0.10975 0.18627
H*11 H 0.69667 0.21320 0.18227
H*12 H 0.67799 -0.01895 0.23589
C1+ C 0.09228 0.80979 -0.06072
N'2+ N 0.02432 0.78841 0.22560
N'3+ N 0.00644 0.73353 0.07413
N'4+ N 0.04875 0.74470 -0.10928
N'5+ N 0.07867 0.83763 0.14494
C6+ C 0.14805 0.84307 -0.22137
N7+ N 0.19531 0.85243 -0.13074
O8+ O 0.22956 0.72079 -0.16902
O9+ O 0.19345 0.99559 -0.02542
N10+ N 0.16168 0.68150 -0.39119
O11+ O 0.16065 0.51663 -0.32861
O12+ O 0.17107 0.73283 -0.57012
N13+ N 0.15515 1.04074 -0.34708
O14+ O 0.11221 1.12152 -0.33987
```

```
O15+ O 0.20362 1.09368 -0.44120

#END

data_FTNM_AGH_3
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 11.790
_cell_length_b                 6.911
_cell_length_c                 7.016
_cell_angle_alpha               88.85
_cell_angle_beta                96.52
_cell_angle_gamma               98.36
_cell_volume                   561.932
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.64844 0.36291 0.23225
N2 N 0.53947 0.38522 0.25272
H*3 H 0.51752 0.51817 0.27539
H*4 H 0.47614 0.26939 0.24601
N5 N 0.73034 0.52108 0.24214
H*6 H 0.70886 0.65504 0.26489
N7 N 0.67724 0.18789 0.20242
H*8 H 0.61826 0.06593 0.19413
H*9 H 0.76096 0.17919 0.18791
N10 N 0.84401 0.49686 0.22066
H*11 H 0.87093 0.57386 0.10473
H*12 H 0.89708 0.54113 0.34144
C1+ C 0.68402 0.10514 -0.26003
N'2+ N 0.55520 0.28723 -0.27103
N'3+ N 0.51030 0.10798 -0.21821
N'4+ N 0.59027 -0.01051 -0.20909
N'5+ N 0.66539 0.29015 -0.29858
C6+ C 0.79334 0.03015 -0.26887
N7+ N 0.89711 0.19525 -0.26522
O8+ O 0.96755 0.21338 -0.12328
O9+ O 0.89802 0.29510 -0.40982
N10+ N 0.81403 -0.11575 -0.10017
O11+ O 0.81531 -0.05068 0.05933
O12+ O 0.82490 -0.28226 -0.14164
N13+ N 0.80164 -0.08969 -0.45651
O14+ O 0.71153 -0.15158 -0.55040
```

```
O15+ O 0.89883 -0.10961 -0.48924

#END

data_FTNM_AGH_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.681
_cell_length_b                 9.897
_cell_length_c                 24.542
_cell_angle_alpha               90.00
_cell_angle_beta               104.75
_cell_angle_gamma               90.00
_cell_volume                   2273.95
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.21083 0.57491 0.07288
N2 N -0.30179 0.57103 0.02162
H*3 H -0.38988 0.62995 0.01179
H*4 H -0.28470 0.50893 -0.00867
N5 N -0.23747 0.65912 0.11207
H*6 H -0.32577 0.71856 0.10247
N7 N -0.09493 0.49734 0.08577
H*8 H -0.07136 0.43295 0.05752
H*9 H -0.02963 0.50424 0.12518
N10 N -0.14208 0.66272 0.16554
H*11 H -0.09944 0.75690 0.17374
H*12 H -0.19269 0.63534 0.19550
C1+ C 0.18590 0.68663 0.09008
N'2+ N 0.02830 0.77391 0.02438
N'3+ N 0.07661 0.66213 0.00481
N'4+ N 0.17626 0.60422 0.04568
N'5+ N 0.09558 0.79218 0.07840
C6+ C 0.28561 0.65896 0.14474
N7+ N 0.24665 0.73626 0.19347
O8+ O 0.20223 0.67271 0.22799
```

```
O9+ O 0.26442 0.85771 0.19238
N10+ N 0.29169 0.50411 0.15708
O11+ O 0.17855 0.45163 0.15705
O12+ O 0.40755 0.44849 0.16460
N13+ N 0.44701 0.70081 0.15018
O14+ O 0.48153 0.71862 0.10665
O15+ O 0.52266 0.71084 0.19811

#END

data_FTNM_AGH_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.946
_cell_length_b                 20.311
_cell_length_c                 6.826
_cell_angle_alpha               90.00
_cell_angle_beta                96.39
_cell_angle_gamma                 90.00
_cell_volume                   1094.81
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.63942 -0.32844 -0.42157
N2 N 0.59519 -0.26510 -0.44700
H*3 H 0.63330 -0.23819 -0.55848
H*4 H 0.52235 -0.24248 -0.35515
N5 N 0.73670 -0.35678 -0.54729
H*6 H 0.77539 -0.33003 -0.65958
N7 N 0.58921 -0.36382 -0.27481
H*8 H 0.51621 -0.34430 -0.17760
H*9 H 0.62628 -0.41155 -0.26226
N10 N 0.78249 -0.42296 -0.51998
H*11 H 0.73703 -0.44995 -0.64010
H*12 H 0.91079 -0.42731 -0.49514
C1+ C 0.27798 0.67050 0.07602
N'2+ N 0.30597 0.76826 0.17576
N'3+ N 0.38339 0.76209 0.01258
N'4+ N 0.36698 0.70063 -0.05459
N'5+ N 0.23775 0.71096 0.21979
C6+ C 0.23185 0.60079 0.05591
```

N7+ N 0.08539 0.58216 0.17643
O8+ O -0.05218 0.56858 0.08873
O9+ O 0.12329 0.58315 0.35391
N10+ N 0.18338 0.58315 -0.16567
O11+ O 0.06864 0.61507 -0.25044
O12+ O 0.26568 0.54017 -0.23597
N13+ N 0.37712 0.54996 0.13014
O14+ O 0.52084 0.57071 0.14861
O15+ O 0.33072 0.49399 0.16144

#END

S18. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidinium 5-(trinitromethyl)tetrazolate (ionic form).

data_FTNM_DAGH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 16.466
_cell_length_b 11.555
_cell_length_c 6.139
_cell_angle_alpha 90.00
_cell_angle_beta 80.03
_cell_angle_gamma 90.00
_cell_volume 1150.4
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.02800 0.34658 0.42703
N2 N 0.02824 0.28758 0.51561
H*3 H 0.00850 0.24380 0.65862
N4 N -0.10728 0.34547 0.52967
H*5 H -0.15033 0.38990 0.46381
N6 N -0.00568 0.40557 0.23973
H*7 H 0.05463 0.40396 0.16828
H*8 H -0.04680 0.45076 0.16940
N9 N -0.12855 0.28256 0.72623
N10 N 0.11058 0.28906 0.40814
H*11 H 0.12958 0.20706 0.36494
H*12 H -0.15248 0.33622 0.85268
H*13 H -0.16989 0.21940 0.70744
H*14 H 0.14695 0.32361 0.50984

```
C1+ C 0.75892 0.02976 -0.06127
N'2+ N 0.63965 0.01155 -0.13579
N'3+ N 0.68179 0.08558 -0.28037
N'4+ N 0.75785 0.09837 -0.23777
N'5+ N 0.68696 -0.02544 0.00541
C6+ C 0.83276 0.01875 0.04043
N7+ N 0.83075 -0.09045 0.18653
O8+ O 0.87820 -0.16936 0.12448
O9+ O 0.77980 -0.08685 0.35526
N10+ N 0.91167 0.01764 -0.14166
O11+ O 0.91423 -0.05776 -0.27993
O12+ O 0.96301 0.09294 -0.13303
N13+ N 0.84790 0.12093 0.20195
O14+ O 0.81153 0.21067 0.18526
O15+ O 0.89547 0.09993 0.32892

#END

data_FTNM_DAGH_2
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 9.515
_cell_length_b                 5.737
_cell_length_c                 11.431
_cell_angle_alpha               96.91
_cell_angle_beta                78.61
_cell_angle_gamma                73.72
_cell_volume                   576.851
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.17052 -0.56424 0.81010
N2 N 0.27752 -0.76089 0.82353
H*3 H 0.30693 -0.91846 0.76073
N4 N 0.10719 -0.58314 0.71525
H*5 H 0.02604 -0.43515 0.70432
N6 N 0.12742 -0.35275 0.88965
H*7 H 0.17814 -0.34700 0.95959
H*8 H 0.04705 -0.20174 0.88169
N9 N 0.15522 -0.80820 0.63341
N10 N 0.34296 -0.74013 0.92232
H*11 H 0.45603 -0.77279 0.89184
H*12 H 0.06752 -0.87660 0.63248
```

H*13 H 0.19969 -0.78549 0.54853
H*14 H 0.32417 -0.86369 0.97559
C1+ C 0.25527 0.78681 0.23212
N'2+ N 0.10674 1.00157 0.14380
N'3+ N 0.24610 0.93008 0.07173
N'4+ N 0.34267 0.79243 0.12519
N'5+ N 0.10885 0.91347 0.24630
C6+ C 0.31872 0.65212 0.32042
N7+ N 0.19714 0.59846 0.41500
O8+ O 0.19607 0.38598 0.41174
O9+ O 0.11085 0.78094 0.48586
N10+ N 0.44333 0.40532 0.25358
O11+ O 0.40326 0.26570 0.18918
O12+ O 0.56994 0.37499 0.26934
N13+ N 0.39984 0.79010 0.40128
O14+ O 0.43668 0.95868 0.36441
O15+ O 0.41853 0.71274 0.49385

#END

data_FTNM_DAGH_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 11.602
_cell_length_b 16.953
_cell_length_c 6.219
_cell_angle_alpha 90.00
_cell_angle_beta 91.65
_cell_angle_gamma 90.00
_cell_volume 1222.7
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.79811 -0.02659 0.74712
N2 N 0.77640 -0.08901 0.87147
H*3 H 0.72847 -0.07997 1.00353
N4 N 0.75613 0.04458 0.80145
H*5 H 0.77214 0.09220 0.70823
N6 N 0.86047 -0.03492 0.57195
H*7 H 0.89029 -0.08954 0.53731
H*8 H 0.87812 0.01112 0.47542

N9 N 0.69094 0.05117 0.98661
N10 N 0.82027 -0.16285 0.81417
H*11 H 0.75426 -0.20160 0.78806
H*12 H 0.73001 0.08872 1.09367
H*13 H 0.60993 0.07051 0.94766
H*14 H 0.87406 -0.18342 0.93372
C1+ C -0.06919 -0.77296 0.45586
N'2+ N -0.10844 -0.89230 0.39791
N'3+ N -0.16622 -0.84849 0.25216
N'4+ N -0.14253 -0.77250 0.28434
N'5+ N -0.04601 -0.84605 0.52948
C6+ C -0.02131 -0.69967 0.54578
N7+ N 0.08766 -0.71396 0.68917
O8+ O 0.18060 -0.69186 0.62560
O9+ O 0.06920 -0.74741 0.85759
N10+ N 0.00663 -0.64094 0.36126
O11+ O 0.07282 -0.66515 0.22920
O12+ O -0.04133 -0.57686 0.36218
N13+ N -0.10389 -0.65167 0.69769
O14+ O -0.20569 -0.66717 0.68386
O15+ O -0.05711 -0.60282 0.81518

#END

data_FTNM_DAGH_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 11.410
_cell_length_b 15.314
_cell_length_c 6.963
_cell_angle_alpha 90.00
_cell_angle_beta 102.82
_cell_angle_gamma 90.00
_cell_volume 1186.34
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.41631 0.44377 0.65058
N2 N 0.31148 0.48649 0.62186
H*3 H 0.23647 0.45440 0.55019
N4 N 0.41797 0.36120 0.58423

H*5 H 0.49696 0.32832 0.60529
N6 N 0.51757 0.48257 0.74364
H*7 H 0.51205 0.54473 0.79100
H*8 H 0.59778 0.45189 0.76725
N9 N 0.30987 0.32246 0.48706
N10 N 0.31031 0.57233 0.69118
H*11 H 0.25737 0.57604 0.79097
H*12 H 0.31371 0.30610 0.34687
H*13 H 0.29254 0.26856 0.56174
H*14 H 0.27850 0.61349 0.57660
C1+ C 0.39575 0.14660 -0.03253
N'2+ N 0.22822 0.10043 -0.18948
N'3+ N 0.27598 0.15037 -0.30989
N'4+ N 0.38263 0.18023 -0.21454
N'5+ N 0.30215 0.09674 -0.01232
C6+ C 0.50325 0.16404 0.12194
N7+ N 0.51931 0.09761 0.29281
O8+ O 0.60168 0.04536 0.31385
O9+ O 0.44497 0.10413 0.39291
N10+ N 0.61729 0.16431 0.03295
O11+ O 0.63493 0.09786 -0.05088
O12+ O 0.67745 0.23094 0.05121
N13+ N 0.50612 0.25588 0.22911
O14+ O 0.43800 0.31135 0.14520
O15+ O 0.57762 0.26255 0.38736

#END

data_FTNM_DAGH_5
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 11.625
_cell_length_b 7.010
_cell_length_c 8.757
_cell_angle_alpha 111.43
_cell_angle_beta 73.16
_cell_angle_gamma 84.67
_cell_volume 619.777
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.09362 0.13302 0.42922
N2 N 0.10735 0.01706 0.26245

H*3 H 0.18354 -0.10191 0.18975
N4 N 0.18015 0.08781 0.49281
H*5 H 0.17055 0.17478 0.61898
N6 N -0.00444 0.29103 0.53072
H*7 H -0.06718 0.31934 0.47736
H*8 H -0.01707 0.38090 0.65684
N9 N 0.28201 -0.07934 0.38245
N10 N 0.01708 0.06481 0.19707
H*11 H -0.02116 -0.06108 0.15678
H*12 H 0.36143 -0.02639 0.36885
H*13 H 0.28461 -0.19075 0.43094
H*14 H 0.05548 0.10289 0.09484
C1+ C 0.22236 0.45314 0.88262
N'2+ N 0.09395 0.47615 1.11759
N'3+ N 0.09944 0.29449 0.98915
N'4+ N 0.18067 0.27513 0.83861
N'5+ N 0.17097 0.58041 1.05411
C6+ C 0.31500 0.49544 0.75216
N7+ N 0.37956 0.66659 0.83631
O8+ O 0.48747 0.61549 0.81765
O9+ O 0.31354 0.84216 0.91649
N10+ N 0.41285 0.28900 0.62002
O11+ O 0.46676 0.20128 0.68403
O12+ O 0.42547 0.23097 0.46548
N13+ N 0.26453 0.58005 0.63310
O14+ O 0.16436 0.55237 0.62720
O15+ O 0.33191 0.66535 0.55697

#END

S19. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidinium 5-(trinitromethyl)tetrazolate (ionic form).

data_FTNM_TAGH_1
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P 21 21 21'
_symmetry_Int_Tables_number 19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 12.635
_cell_length_b 10.097
_cell_length_c 9.823
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1253.18
loop_
_atom_site_label

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.12606 0.89062 0.38645
N2 N -0.21149 0.92893 0.31574
H*3 H -0.20068 0.99648 0.24028
N4 N -0.13594 0.80175 0.48704
H*5 H -0.20954 0.76578 0.50653
N6 N -0.03074 0.94119 0.35657
H*7 H 0.03204 0.90960 0.41254
N8 N -0.04544 0.76333 0.55942
N9 N -0.31023 0.87460 0.34896
H*10 H -0.34052 0.82562 0.26714
H*11 H -0.05406 0.78624 0.65978
H*12 H -0.03365 0.66407 0.54904
H*13 H -0.36093 0.94778 0.37788
N14 N -0.02252 1.03392 0.25097
H*15 H 0.00620 1.12109 0.28780
H*16 H 0.02660 0.99892 0.17706
C1+ C 0.62683 -0.36854 0.03838
N'2+ N 0.50416 -0.34938 0.18168
N'3+ N 0.48411 -0.45509 0.10388
N'4+ N 0.56094 -0.47008 0.01242
N'5+ N 0.59426 -0.29234 0.14264
C6+ C 0.72355 -0.34819 -0.04123
N7+ N 0.80384 -0.25739 0.03202
O8+ O 0.88564 -0.30559 0.07508
O9+ O 0.77618 -0.14237 0.04018
N10+ N 0.77618 -0.48413 -0.07480
O11+ O 0.79870 -0.55212 0.02267
O12+ O 0.78844 -0.51189 -0.19472
N13+ N 0.70794 -0.27894 -0.18509
O14+ O 0.61931 -0.27958 -0.23191
O15+ O 0.78735 -0.23132 -0.23634

#END

data_FTNM_TAGH_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.353
_cell_length_b                 10.256
_cell_length_c                 9.879
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
_cell_volume                   1251.59
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.12008 0.10730 -0.12178
N2 N 0.04003 0.14861 -0.04080
H*3 H -0.03529 0.11196 -0.05723
N4 N 0.22094 0.15256 -0.10446
H*5 H 0.23338 0.21807 -0.02882
N6 N 0.09927 0.02073 -0.22008
H*7 H 0.16215 -0.00813 -0.27929
N8 N 0.30319 0.10786 -0.19043
N9 N 0.06388 0.23912 0.06118
H*10 H 0.04603 0.20054 0.15351
H*11 H 0.33595 0.18415 -0.24216
H*12 H 0.36183 0.06256 -0.13531
H*13 H 0.02015 0.32213 0.04666
N14 N -0.00683 -0.02508 -0.23609
H*15 H -0.03468 -0.00199 -0.33011
H*16 H -0.00880 -0.12358 -0.22327
C1+ C 0.12414 0.62984 0.03644
N'2+ N 0.00709 0.63624 0.19083
N'3+ N -0.01563 0.53582 0.10934
N'4+ N 0.05764 0.52896 0.01078
N'5+ N 0.09541 0.69783 0.14725
C6+ C 0.21763 0.65782 -0.05011
N7+ N 0.30183 0.74613 0.02040
O8+ O 0.38882 0.69956 0.05256
O9+ O 0.27159 0.85765 0.03792
N10+ N 0.27227 0.52807 -0.09636
O11+ O 0.30246 0.45686 -0.00602
O12+ O 0.27831 0.50774 -0.21787
N13+ N 0.19172 0.73304 -0.18694
O14+ O 0.09860 0.73156 -0.22512
O15+ O 0.26863 0.78562 -0.24219

#END

data_FTNM_TAGH_3
_symmetry_cell_setting           monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.505
_cell_length_b 12.368
_cell_length_c 10.495
_cell_angle_alpha 90.00
_cell_angle_beta 65.82
_cell_angle_gamma 90.00
_cell_volume 1243.94
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.17904 0.51246 0.34141
N2 N 0.11539 0.43174 0.30513
H*3 H 0.12813 0.35551 0.33419
N4 N 0.16564 0.61453 0.30568
H*5 H 0.10634 0.62734 0.25111
N6 N 0.25609 0.49111 0.41343
H*7 H 0.30265 0.55454 0.43893
N8 N 0.23321 0.69745 0.34485
N9 N 0.03545 0.45618 0.22987
H*10 H -0.06534 0.43293 0.28518
H*11 H 0.30219 0.73591 0.25829
H*12 H 0.16174 0.75146 0.40742
H*13 H 0.07510 0.41737 0.13606
N14 N 0.26846 0.38375 0.44951
H*15 H 0.37050 0.36077 0.40619
H*16 H 0.23005 0.37632 0.55532
C1+ C 0.18871 0.36719 -0.16452
N'2+ N -0.01437 0.30983 -0.04683
N'3+ N 0.01453 0.29636 -0.18230
N'4+ N 0.14304 0.33156 -0.25949
N'5+ N 0.09419 0.35459 -0.03213
C6+ C 0.32846 0.41351 -0.20662
N7+ N 0.37694 0.41470 -0.08609
O8+ O 0.47093 0.35431 -0.09235
O9+ O 0.31366 0.47803 0.00699
N10+ N 0.43575 0.35011 -0.33386
O11+ O 0.44380 0.25400 -0.31583
O12+ O 0.50009 0.40113 -0.44062
N13+ N 0.34506 0.53591 -0.25688
O14+ O 0.25577 0.57156 -0.29024
O15+ O 0.44743 0.58341 -0.25797

#END

data_FTNM_TAGH_4
_symmetry_cell_setting monoclinic

```
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   7.287
_cell_length_b                   17.512
_cell_length_c                   10.398
_cell_angle_alpha                 90.00
_cell_angle_beta                  67.68
_cell_angle_gamma                    90.00
_cell_volume                     1227.47
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.33829 0.33369 0.77260
N2 N 0.17568 0.32915 0.74203
H*3 H 0.05602 0.36088 0.80003
N4 N 0.50022 0.29302 0.69931
H*5 H 0.49372 0.25943 0.62141
N6 N 0.33897 0.37891 0.87646
H*7 H 0.46513 0.38077 0.89636
N8 N 0.66828 0.29876 0.73331
N9 N 0.17875 0.28147 0.63299
H*10 H 0.15481 0.31281 0.55833
H*11 H 0.70246 0.24662 0.76151
H*12 H 0.78527 0.31883 0.65023
H*13 H 0.07200 0.24061 0.66961
N14 N 0.16785 0.42084 0.95149
H*15 H 0.11619 0.40553 1.05360
H*16 H 0.19901 0.47774 0.94232
C1+ C 0.09911 0.11297 0.82593
N'2+ N -0.11872 0.19554 0.92414
N'3+ N -0.13620 0.17473 0.80559
N'4+ N -0.00046 0.12209 0.74136
N'5+ N 0.02934 0.15730 0.94002
C6+ C 0.26449 0.05905 0.79272
N7+ N 0.31223 0.03837 0.92113
O8+ O 0.27562 -0.02592 0.96877
O9+ O 0.38379 0.09045 0.96390
N10+ N 0.21867 -0.01497 0.72682
O11+ O 0.06831 -0.04839 0.79714
O12+ O 0.33399 -0.03228 0.61044
N13+ N 0.47106 0.08810 0.68271
O14+ O 0.46590 0.14166 0.61053
```

O15+ O 0.61773 0.05341 0.68028

#END

data_FTNM_TAGH_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 12.466
_cell_length_b 11.261
_cell_length_c 10.262
_cell_angle_alpha 90.00
_cell_angle_beta 113.08
_cell_angle_gamma 90.00
_cell_volume 1325.27
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.03822 0.68247 -0.23053
N2 N -0.13429 0.70674 -0.20677
H*3 H -0.18716 0.77274 -0.26473
N4 N 0.03448 0.59626 -0.15696
H*5 H 0.01366 0.55137 -0.08415
N6 N -0.01485 0.74441 -0.32786
H*7 H 0.05884 0.72330 -0.34272
N8 N 0.13430 0.57262 -0.18379
N9 N -0.15675 0.64072 -0.10447
H*10 H -0.23423 0.59728 -0.15027
H*11 H 0.20712 0.58558 -0.09413
H*12 H 0.13235 0.48727 -0.21746
H*13 H -0.15946 0.69559 -0.02694
N14 N -0.09221 0.83407 -0.40333
H*15 H -0.05016 0.91370 -0.38553
H*16 H -0.12494 0.81539 -0.50886
C1+ C -0.01146 0.86416 0.23610
N'2+ N -0.15016 0.98603 0.17880
N'3+ N -0.17406 0.90576 0.07522
N'4+ N -0.08780 0.82692 0.10900
N'5+ N -0.04753 0.96200 0.28248
C6+ C 0.09808 0.80080 0.31214
N7+ N 0.15233 0.83215 0.47143
O8+ O 0.15326 0.75694 0.55718

O9+ O 0.18985 0.93290 0.49640
N10+ N 0.07819 0.66400 0.29303
O11+ O 0.00530 0.62367 0.33150
O12+ O 0.13509 0.60965 0.23920
N13+ N 0.20033 0.82729 0.26046
O14+ O 0.17268 0.87116 0.14412
O15+ O 0.29839 0.80043 0.34299

#END

S20. Optimized crystal structure coordinates for 5 polymorphs of Ammonium 5-nitrotetrazolate 2*N*-oxide (ionic form).

data_T_2O_NH4_1
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P b c a'
_symmetry_Int_Tables_number 61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 11.115
_cell_length_b 8.596
_cell_length_c 11.491
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1097.9
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.08659 0.43228 0.31303
H*2 H 0.16393 0.39302 0.35228
H*3 H 0.03343 0.48697 0.37371
H*4 H 0.10841 0.50945 0.24805
H*5 H 0.04059 0.33968 0.27808
C1+ C 0.19838 0.59616 0.05262
N'2+ N 0.19574 0.64584 -0.05877
N3+ N 0.08267 0.69599 -0.06709
N'4+ N 0.01937 0.67744 0.03516
N'5+ N 0.09459 0.61378 0.11015
O6+ O 0.03666 0.75415 -0.15702
N7+ N 0.30335 0.53014 0.10495

```
O8+ O 0.29754 0.48767 0.20779
O9+ O 0.39513 0.51880 0.04437

#END

data_T_2O_NH4_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.128
_cell_length_b                 8.491
_cell_length_c                 9.006
_cell_angle_alpha               90.00
_cell_angle_beta                63.81
_cell_angle_gamma                90.00
_cell_volume                   557.737
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.34776 0.48846 0.70665
H*2 H -0.24914 0.53050 0.73861
H*3 H -0.43089 0.57961 0.70647
H*4 H -0.28577 0.43906 0.59066
H*5 H -0.42524 0.40466 0.79086
C1+ C 0.04968 0.12818 0.62628
N'2+ N -0.10539 0.18146 0.62351
N3+ N -0.22863 0.14901 0.77739
N'4+ N -0.15131 0.07889 0.86966
N'5+ N 0.02576 0.06673 0.77126
O6+ O -0.39724 0.17787 0.83506
N7+ N 0.22516 0.13663 0.48597
O8+ O 0.36017 0.08478 0.49978
O9+ O 0.23304 0.19569 0.35721

#END

data_T_2O_NH4_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
```

```
_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
_cell_length_a                 6.659
_cell_length_b                 6.960
_cell_length_c                 12.743
_cell_angle_alpha               90.00
_cell_angle_beta                74.76
_cell_angle_gamma                 90.00
_cell_volume                   569.826
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.21236 0.23866 0.65169
H*2 H 0.36157 0.20745 0.60762
H*3 H 0.11153 0.21621 0.60414
H*4 H 0.17204 0.15113 0.71893
H*5 H 0.20431 0.37985 0.67607
C1+ C 0.24669 0.67973 -0.06171
N'2+ N 0.05043 0.73350 -0.01102
N3+ N 0.08224 0.83564 0.07155
N'4+ N 0.28943 0.84343 0.07091
N'5+ N 0.39134 0.74338 -0.01449
O6+ O -0.05815 0.91720 0.14310
N7+ N 0.29619 0.56429 -0.15793
O8+ O 0.48078 0.52182 -0.19897
O9+ O 0.15109 0.51249 -0.19542

#END

data_T_2O_NH4_4
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 9.380
_cell_length_b                 13.534
_cell_length_c                 4.934
_cell_angle_alpha               127.16
_cell_angle_beta                58.89
_cell_angle_gamma                 77.10
_cell_volume                   264.989
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.56831 0.78864 0.52672
H*2 H -0.48494 0.79505 0.60310
H*3 H -0.44449 0.71489 0.11623
H*4 H -0.59108 0.71334 0.49750
H*5 H -0.75273 0.93128 0.89005
C1+ C 0.02930 0.25371 0.39977
N'2+ N -0.03138 0.20302 0.56412
N3+ N -0.21787 0.37146 1.16982
N'4+ N -0.26813 0.51827 1.36449
N'5+ N -0.10887 0.44033 0.86769
O6+ O -0.33760 0.39750 1.53322
N7+ N 0.22504 0.11924 -0.22284
O8+ O 0.26776 0.17862 -0.33121
O9+ O 0.34230 -0.05054 -0.62347

#END

data_T_2O_NH4_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 6.089
_cell_length_b                 7.435
_cell_length_c                 13.498
_cell_angle_alpha               90.00
_cell_angle_beta               102.32
_cell_angle_gamma                90.00
_cell_volume                   597.005
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.31808 0.74655 0.40718
H*2 H 0.41620 0.63609 0.43168
H*3 H 0.41674 0.86003 0.41598
H*4 H 0.24287 0.73089 0.33193
H*5 H 0.19650 0.75918 0.44913
C1+ C 0.15222 0.71789 0.13947
```

N'2+ N 0.03055 0.75134 0.04541
N3+ N -0.13691 0.84922 0.06653
N'4+ N -0.11744 0.87405 0.16926
N'5+ N 0.06754 0.78946 0.21428
O6+ O -0.29671 0.91331 0.00153
N7+ N 0.35494 0.61451 0.15780
O8+ O 0.45570 0.59060 0.24670
O9+ O 0.41954 0.55395 0.08340

#END

S21. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylammonium 5-nitrotetrazolate 2*N*-oxide (ionic form).

data_T_2O_NH3OH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 5.209
_cell_length_b 8.607
_cell_length_c 14.755
_cell_angle_alpha 90.00
_cell_angle_beta 116.93
_cell_angle_gamma 90.00
_cell_volume 589.788
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.26878 0.78914 0.53362
H*2 H 0.29518 0.79764 0.60702
H*3 H 0.05132 0.79089 0.48419
H*4 H 0.37287 0.88132 0.51966
O5 O 0.39536 0.64613 0.53079
H*6 H 0.37484 0.63347 0.46205
C1+ C 0.28318 0.64291 0.28227
N'2+ N 0.12334 0.62608 0.18095
N3+ N -0.09356 0.53990 0.17731
N'4+ N -0.06619 0.50590 0.27259
N'5+ N 0.17480 0.57249 0.33825
O6+ O -0.30229 0.49329 0.09704
N7+ N 0.54665 0.72887 0.32626
O8+ O 0.67924 0.73821 0.42008
O9+ O 0.62897 0.78985 0.26792

```
#END

data_T_2O_NH3OH_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 6.446
_cell_length_b                 6.793
_cell_length_c                 16.302
_cell_angle_alpha               90.00
_cell_angle_beta                60.57
_cell_angle_gamma                90.00
_cell_volume                   621.712
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.07932 0.26498 0.35773
H*2 H 0.19950 0.29758 0.28856
H*3 H 0.05156 0.11469 0.36414
H*4 H 0.14739 0.31314 0.39985
O5 O -0.12838 0.36798 0.37620
H*6 H -0.24763 0.34089 0.44150
C1+ C 0.42479 0.23042 0.10939
N'2+ N 0.46298 0.23732 0.02028
N3+ N 0.27856 0.34589 0.03167
N'4+ N 0.13447 0.40247 0.12396
N'5+ N 0.23061 0.32751 0.17222
O6+ O 0.23658 0.39346 -0.03326
N7+ N 0.57896 0.12788 0.13468
O8+ O 0.53002 0.12940 0.21826
O9+ O 0.75436 0.04241 0.07132

#END

data_T_2O_NH3OH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 5.778
_cell_length_b                 11.788
_cell_length_c                 7.961
_cell_angle_alpha               90.00
_cell_angle_beta                87.13
_cell_angle_gamma                 90.00
_cell_volume                   541.552
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.43297 0.37816 0.38050
H*2 H -0.50341 0.37416 0.50188
H*3 H -0.33075 0.30738 0.35777
H*4 H -0.56585 0.38129 0.29852
O5 O -0.30131 0.47850 0.37561
H*6 H -0.23109 0.48555 0.26193
C1+ C 0.03440 0.64171 0.14522
N'2+ N -0.15460 0.58441 0.09945
N3+ N -0.25749 0.66253 0.00801
N'4+ N -0.13571 0.76309 -0.00123
N'5+ N 0.04931 0.74806 0.08686
O6+ O -0.44460 0.64830 -0.06316
N7+ N 0.20479 0.59291 0.24761
O8+ O 0.37279 0.65183 0.28343
O9+ O 0.17532 0.49371 0.29540

#END

data_T_2O_NH3OH_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.763
_cell_length_b                 6.955
_cell_length_c                 7.600
_cell_angle_alpha               90.00
_cell_angle_beta                109.76
_cell_angle_gamma                 90.00
```

```
_cell_volume                    634.903
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.14803 0.74426 -0.28908
H*2 H 0.13304 0.76494 -0.42977
H*3 H 0.14462 0.59880 -0.26409
H*4 H 0.22557 0.79934 -0.21480
O5 O 0.06240 0.84566 -0.25230
H*6 H 0.07360 0.82967 -0.11951
C1+ C 0.06854 0.79343 0.21613
N'2+ N 0.00450 0.76114 0.03688
N3+ N -0.07464 0.64950 0.06009
N'4+ N -0.05915 0.61554 0.24592
N'5+ N 0.03236 0.70835 0.34280
O6+ O -0.15526 0.58097 -0.07039
N7+ N 0.16697 0.90899 0.26671
O8+ O 0.22067 0.93082 0.43487
O9+ O 0.19354 0.98162 0.13901

#END

data_T_2O_NH3OH_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  7.960
_cell_length_b                  11.790
_cell_length_c                  5.778
_cell_angle_alpha                 90.00
_cell_angle_beta                 87.11
_cell_angle_gamma                   90.00
_cell_volume                    541.566
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.11955 0.37822 0.43298
H*2 H -0.00185 0.37422 0.50347
H*3 H 0.20153 0.38136 0.56584
```

H*4 H 0.14230 0.30746 0.33075
O5 O 0.12443 0.47854 0.30130
H*6 H 0.23813 0.48560 0.23103
C1+ C 0.14519 0.14177 0.03446
N'2+ N 0.09936 0.08449 -0.15451
N3+ N 0.00797 0.16261 -0.25737
N'4+ N -0.00119 0.26317 -0.13561
N'5+ N 0.08691 0.24811 0.04938
O6+ O -0.06323 0.14841 -0.44445
N7+ N 0.24757 0.09294 0.20481
O8+ O 0.28345 0.15184 0.37279
O9+ O 0.29529 -0.00625 0.17534

#END

S22. Optimized crystal structure coordinates for 5 polymorphs of Hydrazinium 5-nitrotetrazolate 2*N*-oxide (ionic form).

data_T_2O_N2H5_1
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P b c a'
_symmetry_Int_Tables_number 61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 11.960
_cell_length_b 8.694
_cell_length_c 12.262
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1275.01
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.61339 -0.03516 0.66764
H*2 H 0.67620 -0.05555 0.61218
H*3 H 0.64726 0.03258 0.72797
N4 N 0.58154 -0.18081 0.71580
H*5 H 0.52007 -0.15936 0.77162
H*6 H 0.54917 -0.24799 0.65517
H*7 H 0.55034 0.02553 0.62943

```
C1+ C -0.77694 0.40944 0.07793
N'2+ N -0.78320 0.36410 -0.02716
N3+ N -0.88960 0.31958 -0.03319
N'4+ N -0.94553 0.33725 0.06432
N'5+ N -0.87239 0.39454 0.13390
O6+ O -0.93584 0.26699 -0.11734
N7+ N -0.67664 0.46855 0.12564
O8+ O -0.67860 0.50741 0.22280
O9+ O -0.59257 0.47786 0.06699

#END

data_T_2O_N2H5_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.598
_cell_length_b                 9.296
_cell_length_c                 12.568
_cell_angle_alpha               90.00
_cell_angle_beta                32.00
_cell_angle_gamma                90.00
_cell_volume                   594.227
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.05836 0.07202 0.25221
H*2 H -0.13578 0.06438 0.37775
H*3 H 0.13970 0.05157 0.13065
N4 N -0.09062 0.21887 0.23692
H*5 H -0.01066 0.22594 0.11074
H*6 H -0.28771 0.23882 0.35925
H*7 H -0.14232 -0.00654 0.25945
C1+ C -0.05994 0.55994 0.26446
N'2+ N 0.00996 0.58296 0.11700
N3+ N -0.19709 0.65653 0.21570
N'4+ N -0.38485 0.67724 0.41493
N'5+ N -0.29379 0.61498 0.44282
O6+ O -0.22318 0.70305 0.13930
N7+ N 0.10230 0.48308 0.23291
O8+ O 0.02226 0.46708 0.37706
O9+ O 0.31560 0.43627 0.06211
```

```
#END

data_T_2O_N2H5_3
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P c a 21'
_symmetry_Int_Tables_number      29
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 11.633
_cell_length_b                 5.670
_cell_length_c                 9.072
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   598.381
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.03819 0.41279 0.46385
H*2 H 0.02557 0.47305 0.39490
H*3 H -0.02022 0.47844 0.56701
N4 N -0.03041 0.15809 0.47037
H*5 H -0.09314 0.09987 0.54028
H*6 H -0.04708 0.09445 0.36720
H*7 H -0.11593 0.48082 0.42900
C1+ C -0.20624 0.98196 0.17161
N'2+ N -0.30835 0.87949 0.14183
N3+ N -0.30308 0.68925 0.22776
N'4+ N -0.20185 0.67700 0.30641
N'5+ N -0.14149 0.86480 0.26911
O6+ O -0.38051 0.53553 0.23798
N7+ N -0.17011 1.19791 0.10459
O8+ O -0.07490 1.27918 0.13853
O9+ O -0.23629 1.29296 0.01561

#END

data_T_2O_N2H5_4
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
```

```
_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
_cell_length_a                10.523
_cell_length_b                12.888
_cell_length_c                8.764
_cell_angle_alpha              90.00
_cell_angle_beta               90.00
_cell_angle_gamma                90.00
_cell_volume                  1188.58
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.62475 0.57591 0.30755
H*2 H 0.68564 0.63828 0.30349
H*3 H 0.67153 0.51794 0.36545
N4 N 0.60286 0.54078 0.15281
H*5 H 0.54348 0.47816 0.15796
H*6 H 0.55767 0.59919 0.09565
H*7 H 0.54494 0.59676 0.36891
C1+ C 0.72537 0.17899 -0.13534
N'2+ N 0.69293 0.27891 -0.11070
N3+ N 0.60214 0.26799 -0.00598
N'4+ N 0.58047 0.16558 0.03129
N'5+ N 0.65981 0.11027 -0.05224
O6+ O 0.54159 0.34152 0.05391
N7+ N 0.82183 0.14893 -0.24146
O8+ O 0.84533 0.05535 -0.25670
O9+ O 0.87715 0.21845 -0.31300

#END

data_T_2O_N2H5_5
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
```

_cell_length_a 9.558
_cell_length_b 9.509
_cell_length_c 6.740
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 612.579
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.67616 0.31019 -0.20047
H*2 H 0.69807 0.24586 -0.31916
H*3 H 0.68108 0.24821 -0.07558
N4 N 0.53385 0.36027 -0.22139
H*5 H 0.51241 0.42275 -0.10189
H*6 H 0.52950 0.42039 -0.34686
H*7 H 0.75267 0.38661 -0.19121
C1+ C 0.69250 0.20353 0.30563
N'2+ N 0.64268 0.14426 0.13797
N3+ N 0.57739 0.03183 0.21101
N'4+ N 0.58727 0.02335 0.41473
N'5+ N 0.66087 0.13354 0.47194
O6+ O 0.51323 -0.05801 0.10892
N7+ N 0.77249 0.33064 0.30577
O8+ O 0.81398 0.37747 0.46681
O9+ O 0.79624 0.38759 0.14393

#END

S23. Optimized crystal structure coordinates for 5 polymorphs of Guanidinium 5-nitrotetrazolate 2*N*-oxide (ionic form).
data_T_2O_GH_1
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P b c a'
_symmetry_Int_Tables_number 61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.204
_cell_length_b 15.351
_cell_length_c 12.312

```
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
_cell_volume                     1361.57
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.10634 0.24493 0.37612
N2 N -0.06587 0.27745 0.37468
H*3 H -0.17822 0.23804 0.37566
H*4 H -0.08867 0.34238 0.37258
N5 N 0.13240 0.15871 0.37891
H*6 H 0.26132 0.13277 0.38004
H*7 H 0.02393 0.11697 0.37997
N8 N 0.25249 0.29864 0.37477
H*9 H 0.23592 0.36399 0.37266
H*10 H 0.38376 0.27544 0.37581
C1+ C 0.26688 -0.00832 0.12520
N'2+ N 0.28352 0.07917 0.12056
N3+ N 0.10599 0.10335 0.12342
N'4+ N -0.01338 0.03332 0.12954
N'5+ N 0.09175 -0.03707 0.13058
O6+ O 0.04992 0.18085 0.12092
N7+ N 0.42337 -0.06564 0.12443
O8+ O 0.39494 -0.14513 0.12895
O9+ O 0.58004 -0.03264 0.11926

#END

data_T_2O_GH_2
_symmetry_cell_setting           monoclinic
_symmetry_space_group_name_H-M   'P 21'
_symmetry_Int_Tables_number      4
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,-z
_cell_length_a                   11.360
_cell_length_b                   15.256
_cell_length_c                   4.854
_cell_angle_alpha                90.00
_cell_angle_beta                 155.89
_cell_angle_gamma                90.00
_cell_volume                     343.637
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.64257 0.68551 -0.35550
N2 N 0.58630 0.77148 -0.47165
H*3 H 0.67859 0.81280 -0.41123
H*4 H 0.44984 0.79763 -0.62324
N5 N 0.82409 0.65270 -0.15527
H*6 H 0.86961 0.58795 -0.06473
H*7 H 0.92105 0.69169 -0.08865
N8 N 0.51732 0.63235 -0.43958
H*9 H 0.37950 0.65578 -0.59054
H*10 H 0.55682 0.56721 -0.35462
C1+ C 0.06712 0.43844 1.16615
N'2+ N 0.07954 0.35042 1.16707
N3+ N -0.10137 0.32547 0.97882
N'4+ N -0.21863 0.39556 0.86831
N'5+ N -0.10867 0.46677 0.99023
O6+ O -0.16204 0.24727 0.90635
N7+ N 0.22840 0.49668 1.33879
O8+ O 0.20366 0.57659 1.32418
O9+ O 0.38530 0.46399 1.49481

#END

data_T_2O_GH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 14.341
_cell_length_b                 7.211
_cell_length_c                 15.338
_cell_angle_alpha               90.00
_cell_angle_beta               120.52
_cell_angle_gamma                90.00
_cell_volume                   1366.39
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

C1 C 0.37313 -0.14205 0.79719
N2 N 0.37045 -0.31380 0.82875
H*3 H 0.37027 -0.33612 0.89371
H*4 H 0.36852 -0.42627 0.78856
N5 N 0.37565 0.00427 0.85192
H*6 H 0.37770 0.13521 0.82946
H*7 H 0.37558 -0.01182 0.91734
N8 N 0.37329 -0.11662 0.71090
H*9 H 0.37142 -0.22523 0.66840
H*10 H 0.37530 0.01194 0.68568
C1+ C 0.12490 -0.01624 0.45559
N'2+ N 0.12721 -0.03417 0.36911
N3+ N 0.12541 0.14291 0.34355
N'4+ N 0.12215 0.26326 0.41181
N'5+ N 0.12188 0.15923 0.48246
O6+ O 0.12650 0.19781 0.26631
N7+ N 0.12563 -0.17179 0.51377
O8+ O 0.12336 -0.14220 0.59221
O9+ O 0.12851 -0.32888 0.48252

#END

data_T_2O_GH_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C c'
_symmetry_Int_Tables_number 9
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 6.244
_cell_length_b 7.204
_cell_length_c 15.831
_cell_angle_alpha 90.00
_cell_angle_beta 74.10
_cell_angle_gamma 90.00
_cell_volume 684.862
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.46181 0.39345 0.43820
N2 N 0.55548 0.36736 0.35236
H*3 H 0.60089 0.47581 0.31081
H*4 H 0.58358 0.23843 0.32654
N5 N 0.42658 0.56567 0.47057
H*6 H 0.35605 0.58850 0.53522

H*7 H 0.46947 0.67801 0.43134
N8 N 0.40337 0.24732 0.49167
H*9 H 0.42849 0.11604 0.46857
H*10 H 0.33238 0.26391 0.55672
N8 N 0.45529 0.52010 0.32970
H*9 H 0.35284 0.58151 0.27170
H*10 H 0.39668 0.44447 0.29835
N'2+ N 0.47940 0.18695 0.33666
N3+ N 0.28296 0.25988 0.35371
C1+ C 0.54333 0.18919 0.54738
N'4+ N 0.23005 0.30450 0.56622
N7+ N 0.24952 0.62306 0.61625
O9+ O 0.37301 0.56148 0.47458
O8+ O 0.29454 0.36953 0.31319
C1+ C 0.21242 0.76637 0.68471
N'2+ N 0.13015 0.78319 0.77257
N3+ N 0.10754 0.60557 0.79680
N'4+ N 0.17345 0.48598 0.72645
N'5+ N 0.23956 0.59105 0.65580
O6+ O 0.03471 0.54961 0.87461
N7+ N 0.26621 0.92286 0.62719
O8+ O 0.34095 0.89427 0.54737
O9+ O 0.23507 1.07972 0.66038
H*7 H 0.44809 0.96724 0.60470
O6+ O 0.15683 0.71351 0.69633
N'5+ N 0.39781 1.25844 0.68676
O8+ O 0.29454 0.63047 0.81319
N'2+ N 0.13015 0.21681 0.27257
N3+ N 0.10754 0.39443 0.2968
O6+ O 0.03471 0.45039 0.37461
O6+ O 0.65683 1.21351 0.69633
N'5+ N -0.10219 0.75844 0.68676

#END

data_T_2O_GH_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 15.353
_cell_length_b 7.203
_cell_length_c 6.205
_cell_angle_alpha 90.00
_cell_angle_beta 91.25
_cell_angle_gamma 90.00

_cell_volume 686.033
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.73551 0.10627 0.75008
N2 N 0.64929 0.13253 0.75099
H*3 H 0.60749 0.02415 0.75143
H*4 H 0.62341 0.26153 0.75128
N5 N 0.76795 -0.06603 0.74972
H*6 H 0.83288 -0.08900 0.74904
H*7 H 0.72848 -0.17831 0.75013
N8 N 0.78929 0.25231 0.74952
H*9 H 0.76616 0.38365 0.74978
H*10 H 0.85464 0.23559 0.74883
C1+ C 0.01806 0.26768 0.24994
N'2+ N -0.06950 0.28441 0.24945
N3+ N -0.09361 0.10674 0.24952
N'4+ N -0.02346 -0.01279 0.25002
N'5+ N 0.04692 0.09237 0.25029
O6+ O -0.17113 0.05069 0.24916
N7+ N 0.07534 0.42425 0.25008
O8+ O 0.15490 0.39573 0.25054
O9+ O 0.04223 0.58108 0.24974

#END

S24. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidinium 5-nitrotetrazolate 2*N*-oxide (ionic form).
data_T_2O_AGH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 15.624
_cell_length_b 6.872
_cell_length_c 7.248
_cell_angle_alpha 90.00
_cell_angle_beta 97.79
_cell_angle_gamma 90.00
_cell_volume 771.023
loop_
_atom_site_label
_atom_site_type_symbol

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.10057 0.36819 -0.57788
N2 N 0.02696 0.26693 -0.58390
H*3 H -0.00023 0.24096 -0.46753
H*4 H -0.00342 0.21364 -0.70528
N5 N 0.13906 0.43674 -0.41324
H*6 H 0.11208 0.41117 -0.29584
N7 N 0.13630 0.40228 -0.73110
H*8 H 0.10936 0.35327 -0.85704
H*9 H 0.19205 0.47972 -0.71875
N10 N 0.21593 0.54241 -0.40783
H*11 H 0.20798 0.67966 -0.35986
H*12 H 0.26468 0.47355 -0.32541
C1+ C 0.12154 0.86767 0.03786
N'2+ N 0.04581 0.79261 -0.04299
N3+ N 0.00600 0.76028 0.10543
N'4+ N 0.05563 0.81361 0.26957
N'5+ N 0.12884 0.88153 0.22350
O6+ O -0.06842 0.68929 0.10021
N7+ N 0.18850 0.92749 -0.06611
O8+ O 0.25593 0.99484 0.01981
O9+ O 0.17551 0.90874 -0.23762

#END

data_T_2O_AGH_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 23.479
_cell_length_b                 8.913
_cell_length_c                 3.797
_cell_angle_alpha               90.00
_cell_angle_beta                84.17
_cell_angle_gamma                 90.00
_cell_volume                   790.482
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.11721 0.22177 0.66796
```

N2 N 0.08696 0.09934 0.77243
H*3 H 0.10590 0.00843 0.86874
H*4 H 0.04428 0.09459 0.75769
N5 N 0.17403 0.22358 0.69193
H*6 H 0.19331 0.13265 0.78843
N7 N 0.09225 0.34134 0.54125
H*8 H 0.04976 0.34419 0.51926
H*9 H 0.11713 0.43105 0.46593
N10 N 0.20540 0.35179 0.58239
H*11 H 0.22417 0.39643 0.78888
H*12 H 0.23565 0.32605 0.37984
C1+ C 0.38672 0.23985 0.85230
N'2+ N 0.35707 0.11510 0.78536
N3+ N 0.30538 0.14935 0.94237
N'4+ N 0.30378 0.28922 1.09815
N'5+ N 0.35595 0.34486 1.03780
O6+ O 0.26220 0.06556 0.95131
N7+ N 0.44613 0.25843 0.73485
O8+ O 0.46989 0.37678 0.80849
O9+ O 0.47086 0.15461 0.56466

#END

data_T_2O_AGH_3
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P c a 21'
_symmetry_Int_Tables_number 29
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 22.907
_cell_length_b 3.813
_cell_length_c 8.802
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 768.805
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.63651 0.44194 0.20431
N2 N 0.66987 0.36395 0.08392
H*3 H 0.65328 0.23880 -0.00759
H*4 H 0.71263 0.42834 0.08139
N5 N 0.57969 0.35153 0.20320

H*6 H 0.56275 0.22579 0.11163
N7 N 0.65838 0.60664 0.32468
H*8 H 0.70076 0.67861 0.32970
H*9 H 0.63122 0.65937 0.41275
N10 N 0.54506 0.43370 0.32927
H*11 H 0.51193 0.59680 0.29820
H*12 H 0.52872 0.21060 0.37666
C1+ C 0.13910 0.07918 0.71841
N'2+ N 0.10481 0.15269 0.59785
N3+ N 0.05516 -0.00251 0.63899
N'4+ N 0.05921 -0.16355 0.77884
N'5+ N 0.11294 -0.10849 0.82738
O6+ O 0.00917 -0.00563 0.56115
N7+ N 0.19848 0.19232 0.72897
O8+ O 0.22670 0.11271 0.84394
O9+ O 0.21872 0.36500 0.62201

#END

data_T_2O_AGH_4
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 7.216
_cell_length_b 8.378
_cell_length_c 12.278
_cell_angle_alpha 57.83
_cell_angle_beta 94.50
_cell_angle_gamma 50.82
_cell_volume 377.363
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.00434 0.32898 0.43267
N2 N 0.19429 0.12050 0.59727
H*3 H 0.36844 0.06290 0.65215
H*4 H 0.16845 0.01497 0.67115
N5 N 0.04663 0.46444 0.33854
H*6 H 0.22112 0.40761 0.39290
N7 N -0.22477 0.40463 0.36056
H*8 H -0.26375 0.30807 0.42698
H*9 H -0.36178 0.56378 0.23552
N10 N -0.15252 0.68203 0.16668
H*11 H -0.26708 0.89439 0.10600

H*12 H -0.03181 0.60601 0.12979
C1+ C 0.02538 -0.15666 0.88738
N'2+ N -0.04474 -0.00754 0.73710
N3+ N -0.26277 0.05729 0.66243
N'4+ N -0.32231 -0.04833 0.76343
N'5+ N -0.13664 -0.18366 0.90590
O6+ O -0.40212 0.19855 0.51642
N7+ N 0.25389 -0.27606 1.01630
O8+ O 0.30308 -0.40981 1.15041
O9+ O 0.39147 -0.23929 0.98696

#END

data_T_2O_AGH_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.349
_cell_length_b 15.124
_cell_length_c 7.163
_cell_angle_alpha 90.00
_cell_angle_beta 74.71
_cell_angle_gamma 90.00
_cell_volume 767.96
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.02994 -0.09998 0.37152
N2 N 0.05312 -0.02545 0.26677
H*3 H 0.17728 0.00735 0.23296
H*4 H -0.05320 0.00003 0.21861
N5 N 0.17524 -0.13177 0.43296
H*6 H 0.30031 -0.09914 0.39950
N7 N -0.13350 -0.14311 0.41593
H*8 H -0.24562 -0.12133 0.37248
H*9 H -0.14345 -0.19920 0.49558
N10 N 0.15018 -0.20965 0.54233
H*11 H 0.24121 -0.25715 0.47246
H*12 H 0.17016 -0.19780 0.67550
C1+ C 0.50415 0.62146 0.37655
N'2+ N 0.58394 0.54510 0.29773
N3+ N 0.43808 0.50594 0.25407

N'4+ N 0.27645 0.55654 0.30443
N'5+ N 0.32152 0.62972 0.38208
O6+ O 0.44347 0.43128 0.17574
N7+ N 0.60620 0.68809 0.44830
O8+ O 0.52144 0.75614 0.51832
O9+ O 0.77496 0.67420 0.43662

#END

S25. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidinium 5-nitrotetrazolate 2*N*-oxide (ionic form).

data_T_2O_DAGH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 13.028
_cell_length_b 4.112
_cell_length_c 17.307
_cell_angle_alpha 90.00
_cell_angle_beta 64.68
_cell_angle_gamma 90.00
_cell_volume 838.087
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.76125 0.72766 0.72436
N2 N 0.74372 0.58733 0.79877
H*3 H 0.80699 0.44671 0.80033
N4 N 0.86061 0.67736 0.65561
H*5 H 0.87466 0.78266 0.59896
N6 N 0.68131 0.91458 0.71853
H*7 H 0.60790 0.94562 0.77187
H*8 H 0.69230 1.02325 0.66324
N9 N 0.94272 0.47953 0.66404
N10 N 0.64024 0.64052 0.87003
H*11 H 0.65444 0.74925 0.91743
H*12 H 0.95982 0.28366 0.62449
H*13 H 1.01501 0.60872 0.65068
H*14 H 0.59938 0.42495 0.89130
C1+ C 0.30993 0.86897 -0.02980
N'2+ N 0.25281 0.65904 -0.05705
N3+ N 0.16398 0.58874 0.01618

N'4+ N 0.16716 0.74961 0.08501
N'5+ N 0.26065 0.92650 0.05438
O6+ O 0.08498 0.39801 0.02344
N7+ N 0.41450 1.01781 -0.08617
O8+ O 0.46105 1.20762 -0.05551
O9+ O 0.45327 0.94875 -0.16314

#END

data_T_2O_DAGH_2
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 9.112
_cell_length_b 7.962
_cell_length_c 8.554
_cell_angle_alpha 107.25
_cell_angle_beta 87.89
_cell_angle_gamma 54.17
_cell_volume 462.435
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.27474 -0.01233 0.01680
N2 N 0.19551 0.16180 0.16663
H*3 H 0.13083 0.31718 0.16525
N4 N 0.26556 0.02512 -0.12752
H*5 H 0.32518 -0.10575 -0.24163
N6 N 0.36148 -0.21986 0.01083
H*7 H 0.36494 -0.24011 0.12255
H*8 H 0.42236 -0.35409 -0.10036
N9 N 0.17331 0.24536 -0.11651
N10 N 0.20551 0.12182 0.31625
H*11 H 0.07344 0.20927 0.39056
H*12 H 0.26431 0.25554 -0.17730
H*13 H 0.06245 0.29481 -0.16772
H*14 H 0.27483 0.17009 0.38099
C1+ C 0.38539 0.70120 0.41999
N'2+ N 0.35166 0.61271 0.27904
N3+ N 0.20584 0.63252 0.34735
N'4+ N 0.15336 0.72913 0.52262
N'5+ N 0.26932 0.77152 0.56622
O6+ O 0.12289 0.57134 0.26421
N7+ N 0.53294 0.71850 0.41376

```
O8+ O 0.55361 0.80213 0.54964
O9+ O 0.63294 0.64856 0.27201

#END

data_T_2O_DAGH_3
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 12.278
_cell_length_b                 3.988
_cell_length_c                 10.597
_cell_angle_alpha               117.49
_cell_angle_beta                75.38
_cell_angle_gamma                83.66
_cell_volume                   429.541
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.75972 0.90386 0.25651
N2 N 0.74983 0.66560 0.12291
H*3 H 0.81802 0.42761 0.04557
N4 N 0.85825 0.81943 0.28251
H*5 H 0.86654 0.99821 0.38338
N6 N 0.67309 1.22026 0.36223
H*7 H 0.60060 1.27225 0.33774
H*8 H 0.67825 1.40473 0.46389
N9 N 0.94752 0.48453 0.16886
N10 N 0.64717 0.75490 0.09653
H*11 H 0.60779 0.53250 0.07584
H*12 H 1.02163 0.56034 0.13639
H*13 H 0.96313 0.29643 0.20620
H*14 H 0.66616 0.79579 0.00620
C1+ C 0.31746 0.30197 0.26872
N'2+ N 0.26866 0.15421 0.16054
N3+ N 0.17630 0.08275 0.23177
N'4+ N 0.16944 0.18318 0.37724
N'5+ N 0.26003 0.32199 0.39847
O6+ O 0.10241 -0.06004 0.17526
N7+ N 0.42192 0.42693 0.24666
O8+ O 0.46050 0.55892 0.35233
O9+ O 0.46864 0.39647 0.12234

#END
```

```
data_T_2O_DAGH_4
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 9.204
_cell_length_b                 6.809
_cell_length_c                 8.481
_cell_angle_alpha               111.28
_cell_angle_beta                84.95
_cell_angle_gamma               106.29
_cell_volume                   475.326
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.26320 0.00450 0.02004
N2 N 0.30144 0.16862 0.16839
H*3 H 0.33865 0.32329 0.16684
N4 N 0.27546 0.05056 -0.12308
H*5 H 0.24675 -0.07269 -0.23607
N6 N 0.21368 -0.20161 0.01436
H*7 H 0.20628 -0.22856 0.12515
H*8 H 0.18410 -0.32838 -0.09572
N9 N 0.32791 0.26901 -0.11242
N10 N 0.28845 0.11972 0.31678
H*11 H 0.21455 0.19379 0.39635
H*12 H 0.42508 0.29127 -0.17873
H*13 H 0.24756 0.31290 -0.15722
H*14 H 0.39166 0.17221 0.37489
C1+ C 0.19232 -0.28396 0.43492
N'2+ N 0.10717 -0.37963 0.29166
N3+ N -0.02704 -0.35117 0.35168
N'4+ N -0.02332 -0.24263 0.52435
N'5+ N 0.11721 -0.20138 0.57479
O6+ O -0.14550 -0.41456 0.26352
N7+ N 0.34983 -0.27173 0.43723
O8+ O 0.41911 -0.18081 0.57465
O9+ O 0.40909 -0.35316 0.30092

#END

data_T_2O_DAGH_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
```

```
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 25.330
_cell_length_b                 3.910
_cell_length_c                 18.088
_cell_angle_alpha               90.00
_cell_angle_beta                69.53
_cell_angle_gamma                 90.00
_cell_volume                   1678.32
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.62146 0.93358 0.36649
N2 N 0.62605 1.08092 0.43078
H*3 H 0.59160 1.20311 0.46811
N4 N 0.57206 0.95315 0.35414
H*5 H 0.56818 0.84232 0.30560
N6 N 0.66523 0.76984 0.31547
H*7 H 0.70156 0.76156 0.32715
H*8 H 0.66292 0.65656 0.26656
N9 N 0.52694 1.12725 0.40897
N10 N 0.67751 1.05972 0.44331
H*11 H 0.67195 0.93694 0.49515
H*12 H 0.51498 1.32825 0.38268
H*13 H 0.49386 0.96549 0.43307
H*14 H 0.69302 1.29885 0.44488
C1+ C 0.65606 0.38549 0.13797
N'2+ N 0.63485 0.36466 0.07927
N3+ N 0.58868 0.55609 0.10840
N'4+ N 0.58219 0.68757 0.18179
N'5+ N 0.62548 0.57602 0.19950
O6+ O 0.55422 0.61430 0.07404
N7+ N 0.70701 0.21792 0.13474
O8+ O 0.72333 0.25125 0.19138
O9+ O 0.73229 0.04723 0.07514

#END
```

S26. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidinium 5-nitrotetrazolate 2*N*-oxide (ionic form).

```
data_T_2O_TAGH_1
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 9.949
_cell_length_b                 8.019
_cell_length_c                 8.704
_cell_angle_alpha               106.36
_cell_angle_beta                126.11
_cell_angle_gamma                96.22
_cell_volume                   503.454
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24346 0.24778 0.26629
N2 N 0.23336 0.26215 0.11027
H*3 H 0.26076 0.16633 0.03823
N4 N 0.20863 0.37058 0.36652
H*5 H 0.17505 0.47250 0.31954
N6 N 0.28839 0.11061 0.32208
H*7 H 0.29457 0.10451 0.44110
N8 N 0.22011 0.35254 0.52906
N9 N 0.18612 0.40676 0.05495
H*10 H 0.07236 0.35353 -0.09827
H*11 H 0.31357 0.46883 0.66639
H*12 H 0.09999 0.33300 0.49251
H*13 H 0.28593 0.48937 0.07560
N14 N 0.32415 -0.01596 0.21486
H*15 H 0.45124 -0.01110 0.31769
H*16 H 0.23767 -0.14694 0.14382
C1+ C 0.34480 0.07652 -0.22008
N'2+ N 0.31687 -0.03441 -0.39239
N3+ N 0.17967 -0.18094 -0.47585
N'4+ N 0.12663 -0.15962 -0.35879
N'5+ N 0.23335 0.00503 -0.19684
O6+ O 0.10459 -0.32425 -0.64241
N7+ N 0.48210 0.25570 -0.07424
O8+ O 0.49801 0.34801 0.07968
O9+ O 0.57849 0.30953 -0.10967

#END
```

```
data_T_2O_TAGH_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.571
_cell_length_b                 12.990
_cell_length_c                 13.488
_cell_angle_alpha               90.00
_cell_angle_beta                138.45
_cell_angle_gamma                90.00
_cell_volume                   996.049
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.22849 0.50577 -0.25537
N2 N 0.12701 0.58170 -0.25165
H*3 H 0.16563 0.65533 -0.25292
N4 N 0.18354 0.40728 -0.25391
H*5 H 0.07156 0.39340 -0.24994
N6 N 0.37493 0.52833 -0.26055
H*7 H 0.44829 0.46858 -0.26325
N8 N 0.29182 0.32933 -0.25787
N9 N -0.02537 0.55609 -0.24626
H*10 H -0.18862 0.58518 -0.33741
H*11 H 0.39334 0.28479 -0.16454
H*12 H 0.16739 0.28491 -0.35051
H*13 H 0.03733 0.58506 -0.15145
N14 N 0.41902 0.63189 -0.26198
H*15 H 0.59372 0.64729 -0.17117
H*16 H 0.36777 0.64741 -0.35714
C1+ C 0.75706 0.13730 0.27132
N'2+ N 0.82423 0.18826 0.22078
N3+ N 0.64410 0.16851 0.07488
N'4+ N 0.47465 0.10802 0.03850
N'5+ N 0.54990 0.08904 0.16501
O6+ O 0.62635 0.20050 -0.02118
N7+ N 0.89565 0.13500 0.42569
O8+ O 0.82011 0.08623 0.46196
O9+ O 1.08506 0.18216 0.51557

#END
```

```
data_T_2O_TAGH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.207
_cell_length_b                 8.385
_cell_length_c                 12.905
_cell_angle_alpha               90.00
_cell_angle_beta                83.75
_cell_angle_gamma                 90.00
_cell_volume                   990.353
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.26828 0.47464 0.50337
N2 N 0.26127 0.36707 0.58061
H*3 H 0.26476 0.40835 0.65436
N4 N 0.26411 0.42654 0.40466
H*5 H 0.25558 0.30751 0.39164
N6 N 0.27947 0.63031 0.52483
H*7 H 0.28450 0.70806 0.46410
N8 N 0.27162 0.54133 0.32534
N9 N 0.24961 0.20507 0.55613
H*10 H 0.15539 0.15940 0.59315
H*11 H 0.36108 0.52136 0.27329
H*12 H 0.17972 0.53665 0.28808
H*13 H 0.33674 0.14411 0.57836
N14 N 0.28361 0.67752 0.62864
H*15 H 0.37905 0.73551 0.63627
H*16 H 0.19770 0.75080 0.65107
C1+ C 0.25934 0.50801 -0.13671
N'2+ N 0.18965 0.39594 -0.18780
N3+ N 0.05212 0.44716 -0.17117
N'4+ N 0.03904 0.58473 -0.11236
N'5+ N 0.17207 0.62141 -0.09127
O6+ O -0.05559 0.37985 -0.20447
N7+ N 0.41370 0.50590 -0.13150
O8+ O 0.46837 0.61372 -0.08284
O9+ O 0.48506 0.39575 -0.17617

#END
```

```
data_T_2O_TAGH_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 21.646
_cell_length_b                 8.579
_cell_length_c                 12.552
_cell_angle_alpha               90.00
_cell_angle_beta                58.12
_cell_angle_gamma                 90.00
_cell_volume                   1979.31
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.38485 0.70344 -0.13503
N2 N 0.38353 0.64691 -0.03427
H*3 H 0.38116 0.52925 -0.02316
N4 N 0.38796 0.85775 -0.15414
H*5 H 0.38923 0.92794 -0.09007
N6 N 0.38306 0.60566 -0.21668
H*7 H 0.38416 0.65313 -0.29186
N8 N 0.38928 0.91389 -0.26017
N9 N 0.38544 0.75155 0.04966
H*10 H 0.43027 0.73106 0.05441
H*11 H 0.34537 0.98367 -0.23337
H*12 H 0.43586 0.97538 -0.31540
H*13 H 0.33979 0.73934 0.13644
N14 N 0.37982 0.44488 -0.19459
H*15 H 0.33366 0.39973 -0.18512
H*16 H 0.42415 0.39145 -0.26715
C1+ C 0.87701 -0.28465 0.01475
N'2+ N 0.84275 -0.15917 0.08706
N3+ N 0.77345 -0.20300 0.14180
N'4+ N 0.76604 -0.34915 0.10416
N'5+ N 0.83254 -0.39902 0.02337
O6+ O 0.71984 -0.12238 0.21937
N7+ N 0.95444 -0.29470 -0.06458
O8+ O 0.98120 -0.41443 -0.12773
```

O9+ O 0.99092 -0.18253 -0.06600

#END

data_T_2O_TAGH_5
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 12.374
_cell_length_b 7.428
_cell_length_c 8.715
_cell_angle_alpha 114.78
_cell_angle_beta 133.46
_cell_angle_gamma 64.61
_cell_volume 515.764
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.76492 0.47749 0.77963
N2 N 0.76179 0.63965 0.92440
H*3 H 0.76568 0.77328 0.92377
N4 N 0.76005 0.29759 0.77356
H*5 H 0.75403 0.29046 0.88142
N6 N 0.77292 0.49523 0.64093
H*7 H 0.77505 0.36874 0.53370
N8 N 0.76347 0.13042 0.62072
N9 N 0.75341 0.61714 1.06759
H*10 H 0.65691 0.70945 1.04744
H*11 H 0.85645 0.01930 0.69618
H*12 H 0.66700 0.07600 0.52159
H*13 H 0.84636 0.65275 1.22204
N14 N 0.77787 0.68491 0.65057
H*15 H 0.87612 0.67537 0.68257
H*16 H 0.68668 0.73207 0.50797
C1+ C -0.23795 0.23148 0.17383
N'2+ N -0.30773 0.16252 -0.03866
N3+ N -0.44497 0.16574 -0.11231
N'4+ N -0.45779 0.23392 0.04908
N'5+ N -0.32489 0.27490 0.22976
O6+ O -0.55263 0.11333 -0.30634
N7+ N -0.08383 0.25618 0.32678
O8+ O -0.02905 0.32046 0.51873
O9+ O -0.01276 0.21176 0.25893

#END

S27. Optimized crystal structure coordinates for 5 polymorphs of Ammonium 5-(trinitromethyl)tetrazolate 2*N*-oxide (ionic form).

```
data_FTNM_2O_NH4_1
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.273
_cell_length_b                 9.059
_cell_length_c                 10.204
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   857.178
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.26513 0.10035 0.00232
H*2 H 0.32029 0.06288 -0.07846
H*3 H 0.32443 0.18117 0.04807
H*4 H 0.16746 0.14305 -0.02650
H*5 H 0.24834 0.01430 0.06617
C1+ C 0.64131 -0.12758 0.20731
N'2+ N 0.47734 -0.15847 0.35016
N3+ N 0.42482 -0.08424 0.24316
N'4+ N 0.52536 -0.06380 0.15103
N'5+ N 0.61466 -0.18598 0.32577
C6+ C 0.77939 -0.13846 0.13835
N7+ N 0.88351 -0.24530 0.20671
O8+ O 0.91758 -0.35861 0.15001
O9+ O 0.92378 -0.20446 0.31418
N10+ N 0.75590 -0.19103 -0.00677
O11+ O 0.68403 -0.30186 -0.01923
O12+ O 0.80898 -0.11635 -0.09374
N13+ N 0.86779 0.01094 0.12432
O14+ O 0.79955 0.12471 0.13194
O15+ O 0.99757 -0.00208 0.10802
O16+ O 0.29667 -0.04111 0.23439

#END
```

```
data_FTNM_2O_NH4_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 10.015
_cell_length_b                 8.636
_cell_length_c                 9.918
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   857.803
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.44004 0.64961 0.39744
H*2 H 0.41237 0.57603 0.32093
H*3 H 0.40342 0.60880 0.48750
H*4 H 0.54244 0.65550 0.40217
H*5 H 0.40194 0.75811 0.37917
C1+ C 0.89571 0.44710 0.37672
N'2+ N 0.71436 0.57442 0.38557
N3+ N 0.70185 0.44866 0.30204
N'4+ N 0.81424 0.36553 0.29493
N'5+ N 0.83767 0.57153 0.43284
C6+ C 1.03178 0.39488 0.40599
N7+ N 1.09343 0.48307 0.52506
O8+ O 1.11822 0.41192 0.62834
O9+ O 1.11282 0.61988 0.50354
N10+ N 1.03352 0.21683 0.43826
O11+ O 0.95485 0.17509 0.52368
O12+ O 1.11095 0.13599 0.37457
N13+ N 1.13681 0.41388 0.28707
O14+ O 1.09206 0.42145 0.17372
O15+ O 1.25394 0.42039 0.32062
O16+ O 0.59618 0.41699 0.24001

#END

data_FTNM_2O_NH4_3
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
```

```
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 10.029
_cell_length_b                 8.442
_cell_length_c                 10.109
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   855.877
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.15000 0.60287 -0.69415
H*2 H -0.15409 0.59118 -0.79528
H*3 H -0.12656 0.71789 -0.67028
H*4 H -0.24107 0.57420 -0.65413
H*5 H -0.07827 0.52821 -0.65691
C1+ C 0.62688 0.19720 -0.64744
N'2+ N 0.63228 0.33007 -0.46899
N3+ N 0.55477 0.19730 -0.45472
N'4+ N 0.54999 0.11055 -0.56527
N'5+ N 0.67800 0.32806 -0.59156
C6+ C 0.65663 0.14367 -0.78204
N7+ N 0.77027 0.23931 -0.84498
O8+ O 0.87485 0.17176 -0.86986
O9+ O 0.74351 0.37771 -0.86520
N10+ N 0.69543 -0.03658 -0.78249
O11+ O 0.78214 -0.07371 -0.70498
O12+ O 0.63498 -0.12355 -0.85790
N13+ N 0.53749 0.15543 -0.88516
O14+ O 0.42562 0.15773 -0.83986
O15+ O 0.56934 0.16237 -1.00156
O16+ O 0.49567 0.16299 -0.34920

#END

data_FTNM_2O_NH4_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 8.857
_cell_length_b 9.279
_cell_length_c 10.484
_cell_angle_alpha 90.00
_cell_angle_beta 95.38
_cell_angle_gamma 90.00
_cell_volume 857.822
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.26059 0.13339 0.50650
H*2 H 0.36380 0.16450 0.47838
H*3 H 0.17896 0.14304 0.43058
H*4 H 0.26663 0.02795 0.53661
H*5 H 0.23297 0.19807 0.58044
C1+ C 0.66271 0.14577 0.21706
N'2+ N 0.51629 0.14896 0.36640
N3+ N 0.44356 0.20033 0.25431
N'4+ N 0.53257 0.19892 0.15813
N'5+ N 0.65501 0.11399 0.34120
C6+ C 0.79469 0.11789 0.14640
N7+ N 0.91455 0.02613 0.22426
O8+ O 0.94037 -0.09483 0.18620
O9+ O 0.97463 0.08562 0.31918
N10+ N 0.74569 0.03919 0.01645
O11+ O 0.66879 -0.06773 0.02521
O12+ O 0.78621 0.09214 -0.08122
N13+ N 0.88432 0.25612 0.10538
O14+ O 0.81463 0.36869 0.09776
O15+ O 1.01656 0.23689 0.08598
O16+ O 0.30877 0.24344 0.24480

#END

data_FTNM_2O_NH4_5
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P 21 21 21'
_symmetry_Int_Tables_number 19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 8.572

_cell_length_b 9.136
_cell_length_c 10.692
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 837.331
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.31870 0.40473 0.49633
H*2 H -0.40971 0.46812 0.52770
H*3 H -0.32298 0.30392 0.53887
H*4 H -0.32731 0.39185 0.40108
H*5 H -0.21480 0.45503 0.51767
C1+ C 0.14519 0.37509 0.21186
N'2+ N -0.02248 0.34444 0.35588
N3+ N -0.08976 0.40579 0.25195
N'4+ N 0.01272 0.42572 0.15924
N'5+ N 0.12647 0.32481 0.32888
C6+ C 0.29160 0.36848 0.14149
N7+ N 0.41510 0.27548 0.20850
O8+ O 0.45756 0.16158 0.15961
O9+ O 0.46061 0.32688 0.30687
N10+ N 0.26325 0.30372 0.00732
O11+ O 0.19341 0.18844 0.00451
O12+ O 0.31076 0.37432 -0.08170
N13+ N 0.37512 0.52091 0.11629
O14+ O 0.29342 0.62911 0.11978
O15+ O 0.51524 0.51570 0.09646
O16+ O -0.23158 0.43889 0.24617

#END

S28. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylammonium 5-(trinitromethyl)tetrazolate 2*N*-oxide (ionic form).
data_FTNM_2O_NH3OH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.706
_cell_length_b 9.009
_cell_length_c 11.234

```
_cell_angle_alpha                90.00
_cell_angle_beta                 58.05
_cell_angle_gamma                90.00
_cell_volume                    919.381
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.28169 0.82519 -0.69517
H*2 H 0.27743 0.81219 -0.78411
H*3 H 0.33994 0.92066 -0.70519
H*4 H 0.17555 0.83192 -0.60911
O5 O 0.35455 0.69748 -0.69063
H*6 H 0.36094 0.70543 -0.60730
C1+ C 0.12289 0.27473 0.70566
N'2+ N -0.04178 0.31406 0.91928
N3+ N -0.09764 0.23423 0.85381
N'4+ N 0.00367 0.20687 0.71922
N'5+ N 0.09847 0.33830 0.82423
C6+ C 0.26639 0.26849 0.57411
N7+ N 0.39127 0.32090 0.59300
O8+ O 0.48409 0.23102 0.57723
O9+ O 0.38549 0.45177 0.62208
N10+ N 0.30066 0.10627 0.51371
O11+ O 0.28789 0.01077 0.59540
O12+ O 0.33457 0.08940 0.39243
N13+ N 0.28286 0.36670 0.44909
O14+ O 0.17016 0.39932 0.45445
O15+ O 0.40821 0.40180 0.35868
O16+ O -0.22921 0.19257 0.91484

#END

data_FTNM_2O_NH3OH_2
_symmetry_cell_setting           orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  17.955
_cell_length_b                  10.704
```

```
_cell_length_c                  9.605
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                  90.00
_cell_volume                    1845.99
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.92469 0.92882 0.68175
H*2 H 0.89665 0.99088 0.74485
H*3 H 0.88676 0.88516 0.61715
H*4 H 0.96382 0.97727 0.62432
O5 O 0.95820 0.84413 0.77444
H*6 H 0.98553 0.78329 0.71848
C1+ C 0.11704 0.60305 -0.53384
N'2+ N 0.05098 0.70128 -0.38651
N3+ N 0.06022 0.77028 -0.50560
N'4+ N 0.10125 0.71061 -0.60083
N'5+ N 0.08699 0.59509 -0.40617
C6+ C 0.15919 0.50293 -0.60158
N7+ N 0.15472 0.37988 -0.51997
O8+ O 0.12273 0.29132 -0.57303
O9+ O 0.18499 0.38282 -0.40675
N10+ N 0.12979 0.48027 -0.75351
O11+ O 0.06315 0.46475 -0.76349
O12+ O 0.17532 0.48196 -0.84773
N13+ N 0.24582 0.52752 -0.62110
O14+ O 0.26588 0.63564 -0.62128
O15+ O 0.28485 0.43479 -0.63320
O16+ O 0.03292 0.87717 -0.52158

#END

data_FTNM_2O_NH3OH_3
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  10.543
_cell_length_b                  9.448
_cell_length_c                  9.179
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
```

```
_cell_angle_gamma              90.00
_cell_volume                  914.323
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.27240 0.12511 -0.00141
H*2 H 0.33640 0.05005 0.03370
H*3 H 0.32043 0.21826 -0.02211
H*4 H 0.22823 0.08841 -0.09449
O5 O 0.18657 0.13984 0.11483
H*6 H 0.12388 0.21053 0.08582
C1+ C 0.04731 0.62653 -0.11656
N'2+ N -0.09079 0.59666 -0.28233
N3+ N 0.00994 0.67400 -0.33341
N'4+ N 0.09896 0.69395 -0.23173
N'5+ N -0.06549 0.56659 -0.14480
C6+ C 0.11518 0.61423 0.02207
N7+ N 0.05319 0.50549 0.12387
O8+ O 0.11196 0.39817 0.15398
O9+ O -0.05187 0.53872 0.16658
N10+ N 0.25711 0.57074 -0.00433
O11+ O 0.27240 0.46761 -0.08084
O12+ O 0.33908 0.64404 0.05135
N13+ N 0.12433 0.75482 0.11645
O14+ O 0.11282 0.86580 0.05156
O15+ O 0.14129 0.73856 0.24692
O16+ O 0.01625 0.72009 -0.46134

#END

data_FTNM_2O_NH3OH_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.236
_cell_length_b                 8.688
_cell_length_c                 11.370
_cell_angle_alpha               90.00
_cell_angle_beta                92.30
_cell_angle_gamma              90.00
_cell_volume                  911.621
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.24578 0.66625 0.43992
H*2 H 0.24383 0.67683 0.34959
H*3 H 0.14100 0.67377 0.46796
H*4 H 0.29139 0.56143 0.46304
O5 O 0.33159 0.79006 0.48129
H*6 H 0.33623 0.78425 0.56714
C1+ C 0.13877 0.28178 0.27676
N'2+ N -0.01506 0.32165 0.40743
N3+ N -0.07649 0.24200 0.31398
N'4+ N 0.01793 0.21428 0.23042
N'5+ N 0.12177 0.34540 0.38292
C6+ C 0.27636 0.27475 0.21731
N7+ N 0.40458 0.32530 0.29829
O8+ O 0.49637 0.23005 0.32708
O9+ O 0.40225 0.46040 0.32617
N10+ N 0.30530 0.10718 0.17203
O11+ O 0.29572 0.00650 0.24506
O12+ O 0.33240 0.09179 0.06858
N13+ N 0.28722 0.37922 0.10331
O14+ O 0.17391 0.41590 0.05358
O15+ O 0.40938 0.41450 0.07621
O16+ O -0.20674 0.20080 0.30887

#END

data_FTNM_2O_NH3OH_5
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.929
_cell_length_b                 9.786
_cell_length_c                 9.500
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   923.069
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.21436 0.63805 -0.47014
H*2 H 0.17835 0.71849 -0.52920
H*3 H 0.20388 0.54897 -0.52743
H*4 H 0.31434 0.65594 -0.44640
O5 O 0.13345 0.63736 -0.34870
H*6 H 0.16445 0.56211 -0.28945
C1+ C 0.13752 0.87183 0.20315
N'2+ N -0.03128 0.85824 0.33992
N3+ N -0.06225 0.93250 0.22181
N'4+ N 0.04185 0.94225 0.13312
N'5+ N 0.09559 0.81975 0.32632
C6+ C 0.27111 0.84893 0.14225
N7+ N 0.35065 0.73993 0.22338
O8+ O 0.37737 0.63271 0.16411
O9+ O 0.38086 0.77280 0.34273
N10+ N 0.25910 0.80390 -0.01595
O11+ O 0.18365 0.70893 -0.03785
O12+ O 0.32381 0.86817 -0.10270
N13+ N 0.36807 0.97802 0.13803
O14+ O 0.31471 1.08935 0.14161
O15+ O 0.48849 0.95355 0.13260
O16+ O -0.17588 0.98473 0.20108

#END
```

S29. Optimized crystal structure coordinates for 5 polymorphs of Hydrazinium 5-(trinitromethyl)tetrazolate 2*N*-oxide (ionic form).

```
data_FTNM_2O_N2H5_1
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.090
_cell_length_b                 9.769
_cell_length_c                 10.671
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   947.587
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

```
_atom_site_fract_z
N1 N 0.25741 0.13619 0.47039
H*2 H 0.33147 0.18286 0.52944
H*3 H 0.22849 0.20784 0.40418
N4 N 0.12733 0.10231 0.54233
H*5 H 0.05374 0.05744 0.48275
H*6 H 0.15730 0.03232 0.60873
H*7 H 0.30909 0.05545 0.42606
C1+ C 0.12913 0.37847 0.19845
N'2+ N -0.03629 0.34539 0.33585
N3+ N -0.08878 0.42453 0.23954
N'4+ N 0.01262 0.44656 0.15106
N'5+ N 0.10189 0.31628 0.30822
C6+ C 0.26789 0.36822 0.12936
N7+ N 0.37068 0.25988 0.18579
O8+ O 0.39917 0.15827 0.12391
O9+ O 0.41580 0.28750 0.29006
N10+ N 0.23855 0.33202 -0.01186
O11+ O 0.16014 0.23355 -0.02937
O12+ O 0.29411 0.40569 -0.09109
N13+ N 0.36430 0.50373 0.12373
O14+ O 0.29997 0.61103 0.13950
O15+ O 0.49561 0.48769 0.10487
O16+ O -0.21763 0.47030 0.23637

#END

data_FTNM_2O_N2H5_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.355
_cell_length_b                 8.715
_cell_length_c                 11.526
_cell_angle_alpha               90.00
_cell_angle_beta                91.32
_cell_angle_gamma                 90.00
_cell_volume                   939.452
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.25640 -0.16264 0.55837
```

H*2 H 0.26049 -0.17900 0.64677
H*3 H 0.23848 -0.04748 0.54494
N4 N 0.13448 -0.24633 0.51145
H*5 H 0.13024 -0.22810 0.42388
H*6 H 0.15237 -0.36037 0.52629
H*7 H 0.35451 -0.19106 0.52512
C1+ C 0.63383 -0.20762 0.26322
N'2+ N 0.48578 -0.17406 0.39798
N3+ N 0.42390 -0.25344 0.30717
N'4+ N 0.51473 -0.27722 0.22111
N'5+ N 0.61923 -0.14645 0.36919
C6+ C 0.76754 -0.21007 0.19963
N7+ N 0.89543 -0.15776 0.27549
O8+ O 0.98888 -0.25080 0.29971
O9+ O 0.89112 -0.02367 0.30441
N10+ N 0.79819 -0.37555 0.15228
O11+ O 0.79338 -0.47736 0.22368
O12+ O 0.82178 -0.38843 0.04910
N13+ N 0.77216 -0.10376 0.08779
O14+ O 0.65810 -0.06929 0.04310
O15+ O 0.89083 -0.06500 0.05708
O16+ O 0.29633 -0.29776 0.30633

#END

data_FTNM_2O_N2H5_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.822
_cell_length_b 8.954
_cell_length_c 11.184
_cell_angle_alpha 90.00
_cell_angle_beta 121.38
_cell_angle_gamma 90.00
_cell_volume 925.217
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.27099 -0.17642 -0.07265
H*2 H -0.26542 -0.15969 0.02103
H*3 H -0.32900 -0.08841 -0.13650

N4 N -0.35217 -0.31216 -0.13491
H*5 H -0.35859 -0.32705 -0.22856
H*6 H -0.29465 -0.39874 -0.07012
H*7 H -0.16744 -0.17342 -0.05518
C1+ C 0.12597 -0.22537 0.83618
N'2+ N -0.03307 -0.18251 0.88892
N3+ N -0.09003 -0.26508 0.76825
N'4+ N 0.00776 -0.29470 0.73266
N'5+ N 0.10428 -0.15880 0.93130
C6+ C 0.26577 -0.23319 0.84522
N7+ N 0.39031 -0.17853 0.98755
O8+ O 0.48221 -0.26823 1.06511
O9+ O 0.38523 -0.04624 1.00929
N10+ N 0.29849 -0.39744 0.82048
O11+ O 0.28754 -0.49165 0.89221
O12+ O 0.32957 -0.41698 0.73130
N13+ N 0.27946 -0.13727 0.73314
O14+ O 0.16757 -0.10565 0.62618
O15+ O 0.40211 -0.10270 0.76527
O16+ O -0.21949 -0.30704 0.70023

#END

data_FTNM_2O_N2H5_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 11.299
_cell_length_b 13.903
_cell_length_c 5.763
_cell_angle_alpha 90.00
_cell_angle_beta 81.81
_cell_angle_gamma 90.00
_cell_volume 896.076
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.27582 -0.03257 -0.16681
H*2 H -0.25755 -0.03619 -0.34663
H*3 H -0.33078 0.02595 -0.12793
N4 N -0.16472 -0.01441 -0.07643
H*5 H -0.18383 -0.00984 0.10191

H*6 H -0.11018 -0.07234 -0.11804
H*7 H -0.32162 -0.09391 -0.10585
C1+ C 0.48475 0.81638 0.57433
N'2+ N 0.42600 0.91939 0.83812
N3+ N 0.37522 0.93627 0.63952
N'4+ N 0.40993 0.87222 0.47043
N'5+ N 0.49480 0.84278 0.79474
C6+ C 0.54187 0.73147 0.45673
N7+ N 0.59853 0.66673 0.62651
O8+ O 0.55681 0.58665 0.66875
O9+ O 0.68287 0.70282 0.70379
N10+ N 0.44884 0.67097 0.33994
O11+ O 0.35766 0.65071 0.46795
O12+ O 0.47448 0.65085 0.13288
N13+ N 0.64678 0.75203 0.24826
O14+ O 0.64665 0.83011 0.15477
O15+ O 0.71919 0.68727 0.20150
O16+ O 0.30445 1.00447 0.62146

#END

data_FTNM_2O_N2H5_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 9.252
_cell_length_b 8.506
_cell_length_c 11.725
_cell_angle_alpha 90.00
_cell_angle_beta 100.07
_cell_angle_gamma 90.00
_cell_volume 908.514
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.24433 0.18566 0.47723
H*2 H 0.27514 0.19057 0.56582
H*3 H 0.25622 0.07056 0.45363
N4 N 0.34607 0.28055 0.42596
H*5 H 0.31572 0.27364 0.33804
H*6 H 0.33475 0.39434 0.45086
H*7 H 0.13492 0.21628 0.45589

C1+ C 0.13869 0.81502 0.26956
N'2+ N 0.00326 0.86723 0.39348
N3+ N -0.06874 0.77173 0.30767
N'4+ N 0.01403 0.73594 0.22857
N'5+ N 0.13505 0.89308 0.36853
C6+ C 0.26732 0.80501 0.21274
N7+ N 0.40549 0.87172 0.28897
O8+ O 0.50613 0.78213 0.32494
O9+ O 0.40107 1.01253 0.30600
N10+ N 0.29718 0.62988 0.18132
O11+ O 0.30363 0.53694 0.26038
O12+ O 0.30905 0.60153 0.08140
N13+ N 0.25566 0.89640 0.09330
O14+ O 0.13307 0.92296 0.04115
O15+ O 0.37186 0.93308 0.06486
O16+ O -0.19769 0.72449 0.30499

#END

S30. Optimized crystal structure coordinates for 5 polymorphs of Guanidinium 5-(trinitromethyl)tetrazolate 2*N*-oxide (ionic form).

data_FTNM_2O_GH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 11.506
_cell_length_b 14.481
_cell_length_c 7.159
_cell_angle_alpha 90.00
_cell_angle_beta 115.92
_cell_angle_gamma 90.00
_cell_volume 1072.83
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.38579 0.60971 -0.07701
N2 N -0.51143 0.63065 -0.15451
H*3 H -0.56577 0.63858 -0.30887
H*4 H -0.55570 0.63916 -0.06096
N5 N -0.32972 0.59885 -0.20449
H*6 H -0.23494 0.58302 -0.14921
H*7 H -0.38051 0.60615 -0.35984

N8 N -0.31622 0.59963 0.12797
H*9 H -0.35666 0.60753 0.22705
H*10 H -0.22116 0.58382 0.18978
C1+ C 0.26230 0.12180 0.73080
N'2+ N 0.15698 0.13633 0.90991
N3+ N 0.07662 0.11218 0.70913
N'4+ N 0.14021 0.10196 0.59256
N'5+ N 0.27464 0.14171 0.92176
C6+ C 0.37018 0.11538 0.67485
N7+ N 0.50148 0.11873 0.86657
O8+ O 0.57007 0.05024 0.91057
O9+ O 0.52524 0.19217 0.95818
N10+ N 0.36143 0.02375 0.55201
O11+ O 0.34894 -0.04622 0.63430
O12+ O 0.36584 0.03031 0.38536
N13+ N 0.37784 0.19453 0.52693
O14+ O 0.27814 0.23479 0.42141
O15+ O 0.48428 0.20837 0.53378
O16+ O -0.04285 0.10125 0.64470

#END

data_FTNM_2O_GH_2
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 11.604
_cell_length_b 7.949
_cell_length_c 7.062
_cell_angle_alpha 106.23
_cell_angle_beta 115.72
_cell_angle_gamma 67.91
_cell_volume 538.482
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.16774 -0.22090 0.40456
N2 N 0.23999 -0.22734 0.61157
H*3 H 0.20449 -0.24947 0.70737
H*4 H 0.33221 -0.21027 0.67825
N5 N 0.04597 -0.24397 0.32058
H*6 H -0.01029 -0.23962 0.16457
H*7 H 0.00667 -0.26643 0.41067
N8 N 0.21725 -0.19139 0.28153

H*9 H 0.30902 -0.17361 0.34174
H*10 H 0.16434 -0.18601 0.12476
C1+ C 0.20310 0.24438 1.25961
N'2+ N 0.09047 0.27353 1.44311
N3+ N 0.02552 0.21645 1.23330
N'4+ N 0.09432 0.19575 1.11365
N'5+ N 0.20336 0.28975 1.45771
C6+ C 0.31290 0.23488 1.20278
N7+ N 0.43818 0.25272 1.39952
O8+ O 0.53857 0.12120 1.43017
O9+ O 0.42463 0.40195 1.50858
N10+ N 0.35044 0.04935 1.05830
O11+ O 0.37143 -0.08762 1.12648
O12+ O 0.35343 0.05789 0.89077
N13+ N 0.28341 0.38800 1.06997
O14+ O 0.16691 0.46044 0.97046
O15+ O 0.38119 0.42036 1.08119
O16+ O -0.08585 0.18768 1.16416

#END

data_FTNM_2O_GH_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 15.828
_cell_length_b 7.207
_cell_length_c 9.834
_cell_angle_alpha 90.00
_cell_angle_beta 113.44
_cell_angle_gamma 90.00
_cell_volume 1029.21
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.47852 -0.40916 0.27476
N2 N 0.45835 -0.23853 0.30624
H*3 H 0.49477 -0.17853 0.40528
H*4 H 0.40609 -0.16461 0.23190
N5 N 0.54807 -0.50381 0.37528
H*6 H 0.56448 -0.63290 0.35377
H*7 H 0.58626 -0.44901 0.47567

N8 N 0.42914 -0.48514 0.14276
H*9 H 0.37631 -0.41605 0.06522
H*10 H 0.44322 -0.61386 0.11670
C1+ C 0.24683 -0.19069 0.76638
N'2+ N 0.17437 -0.41862 0.80568
N3+ N 0.11884 -0.31969 0.68367
N'4+ N 0.16266 -0.17573 0.65546
N'5+ N 0.25554 -0.33580 0.85659
C6+ C 0.32181 -0.06442 0.77759
N7+ N 0.41547 -0.13434 0.88859
O8+ O 0.47329 -0.17990 0.84204
O9+ O 0.42317 -0.13644 1.01666
N10+ N 0.32658 -0.03836 0.62223
O11+ O 0.32887 -0.18078 0.55828
O12+ O 0.32620 0.11999 0.57819
N13+ N 0.31389 0.14098 0.83005
O14+ O 0.23743 0.19433 0.81135
O15+ O 0.38601 0.22696 0.88591
O16+ O 0.03639 -0.36141 0.60838

#END

data_FTNM_2O_GH_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.736
_cell_length_b 13.067
_cell_length_c 11.257
_cell_angle_alpha 90.00
_cell_angle_beta 102.16
_cell_angle_gamma 90.00
_cell_volume 1112.4
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.07885 0.37588 0.11969
N2 N -0.03342 0.31983 0.03870
H*3 H -0.04052 0.32771 -0.05151
H*4 H -0.11443 0.26796 0.06533
N5 N 0.18454 0.44397 0.08184
H*6 H 0.27033 0.48710 0.14150

H*7 H 0.18171 0.45429 -0.00751
N8 N 0.08543 0.36384 0.23853
H*9 H 0.00674 0.31283 0.26908
H*10 H 0.16927 0.40540 0.30125
C1+ C 0.48875 -0.09836 0.83117
N'2+ N 0.30262 -0.19466 0.89081
N3+ N 0.23977 -0.16302 0.77348
N'4+ N 0.35449 -0.10268 0.73299
N'5+ N 0.46114 -0.15351 0.92606
C6+ C 0.65247 -0.04316 0.82800
N7+ N 0.80054 -0.06918 0.93764
O8+ O 0.93055 -0.11465 0.91997
O9+ O 0.77296 -0.04031 1.03467
N10+ N 0.71744 -0.06844 0.70817
O11+ O 0.72891 -0.15876 0.68667
O12+ O 0.74799 0.00342 0.64656
N13+ N 0.63984 0.07818 0.82865
O14+ O 0.49431 0.11507 0.79343
O15+ O 0.77840 0.12381 0.86564
O16+ O 0.09110 -0.18847 0.71241

#END

data_FTNM_2O_GH_5
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 11.505
_cell_length_b 7.177
_cell_length_c 7.712
_cell_angle_alpha 93.57
_cell_angle_beta 76.57
_cell_angle_gamma 64.49
_cell_volume 549.358
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.16295 -0.51917 0.71165
N2 N -0.21258 -0.65225 0.68315
H*3 H -0.16263 -0.80590 0.68916
H*4 H -0.30148 -0.60306 0.65476
N5 N -0.04503 -0.58864 0.74897
H*6 H -0.00571 -0.49077 0.77095
H*7 H 0.00820 -0.74104 0.75627

N8 N -0.23124 -0.31662 0.70284
H*9 H -0.32051 -0.26085 0.67484
H*10 H -0.19557 -0.21341 0.72392
C1+ C 0.20598 -0.16745 0.74368
N'2+ N 0.08941 -0.33255 0.77722
N3+ N 0.02281 -0.14425 0.72631
N'4+ N 0.09399 -0.03698 0.70306
N'5+ N 0.20582 -0.34574 0.78676
C6+ C 0.31899 -0.11936 0.72872
N7+ N 0.44607 -0.31029 0.73801
O8+ O 0.54336 -0.38785 0.60372
O9+ O 0.43705 -0.36654 0.88396
N10+ N 0.35155 -0.04153 0.54620
O11+ O 0.36666 -0.15449 0.41070
O12+ O 0.35692 0.12474 0.55545
N13+ N 0.29658 0.06240 0.88087
O14+ O 0.18112 0.18813 0.95873
O15+ O 0.39818 0.05846 0.90706
O16+ O -0.09193 -0.08205 0.70476

#END

S31. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidinium 5-(trinitromethyl)tetrazolate 2*N*-oxide (ionic form).

data_FTNM_2O_AGH_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 11.950
_cell_length_b 7.168
_cell_length_c 7.043
_cell_angle_alpha 93.11
_cell_angle_beta 101.28
_cell_angle_gamma 84.34
_cell_volume 588.37
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.12841 0.75856 -0.15179
N2 N 0.01452 0.76076 -0.17088
H*3 H -0.02235 0.74655 -0.05565
H*4 H -0.03772 0.77674 -0.30137
N5 N 0.19505 0.73695 0.02473
H*6 H 0.15855 0.72260 0.14106

N7 N 0.17685 0.77728 -0.30351
H*8 H 0.12974 0.79376 -0.43809
H*9 H 0.26344 0.77462 -0.28101
N10 N 0.31396 0.73476 0.04377
H*11 H 0.34362 0.84240 0.13402
H*12 H 0.35300 0.60981 0.09513
C1+ C 0.20478 0.26207 0.64942
N'2+ N 0.11037 0.27196 0.87656
N3+ N 0.04513 0.21644 0.70400
N'4+ N 0.10243 0.20776 0.55816
N'5+ N 0.21169 0.29946 0.84000
C6+ C 0.29998 0.26597 0.54701
N7+ N 0.41410 0.28694 0.68728
O8+ O 0.48893 0.15717 0.69724
O9+ O 0.41897 0.43669 0.77696
N10+ N 0.31207 0.08232 0.41771
O11+ O 0.31673 -0.06303 0.50026
O12+ O 0.31402 0.10030 0.24720
N13+ N 0.28893 0.43080 0.40064
O14+ O 0.19301 0.50048 0.33866
O15+ O 0.37860 0.47393 0.36444
O16+ O -0.05669 0.17874 0.68742

#END

data_FTNM_2O_AGH_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 14.052
_cell_length_b 7.738
_cell_length_c 14.141
_cell_angle_alpha 90.00
_cell_angle_beta 128.10
_cell_angle_gamma 90.00
_cell_volume 1210
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.14723 0.76953 -0.24894
N2 N 0.02910 0.80438 -0.31239
H*3 H -0.01322 0.79493 -0.27523

H*4 H -0.02098 0.84114 -0.39934
N5 N 0.21080 0.72091 -0.13323
H*6 H 0.16882 0.71118 -0.09537
N7 N 0.20285 0.78200 -0.29792
H*8 H 0.15824 0.81804 -0.38437
H*9 H 0.29239 0.75414 -0.24589
N10 N 0.33416 0.68469 -0.06741
H*11 H 0.38394 0.76645 0.00399
H*12 H 0.35126 0.55970 -0.03872
C1+ C 0.19298 0.28986 0.64595
N'2+ N 0.09213 0.29485 0.71199
N3+ N 0.02887 0.21238 0.60303
N'4+ N 0.09031 0.20621 0.55934
N'5+ N 0.19638 0.34252 0.73845
C6+ C 0.29284 0.30865 0.63994
N7+ N 0.40954 0.36925 0.76001
O8+ O 0.49576 0.27098 0.81506
O9+ O 0.40446 0.51486 0.78901
N10+ N 0.31807 0.13298 0.60338
O11+ O 0.33151 0.00903 0.66291
O12+ O 0.32026 0.13480 0.51849
N13+ N 0.27198 0.44308 0.54382
O14+ O 0.16795 0.47663 0.46026
O15+ O 0.36310 0.50206 0.56318
O16+ O -0.07486 0.15059 0.55141

#END

data_FTNM_2O_AGH_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.273
_cell_length_b 9.721
_cell_length_c 22.916
_cell_angle_alpha 90.00
_cell_angle_beta 92.10
_cell_angle_gamma 90.00
_cell_volume 2286.94
loop_
_atom_site_label

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25661 -0.04364 0.43950
N2 N 0.27915 -0.04038 0.49744
H*3 H 0.35463 -0.09201 0.51659
H*4 H 0.22114 0.01394 0.52362
N5 N 0.33626 -0.11730 0.40613
H*6 H 0.41225 -0.16939 0.42509
N7 N 0.15725 0.02434 0.41434
H*8 H 0.09544 0.08067 0.43789
H*9 H 0.14459 0.01840 0.37031
N10 N 0.31222 -0.12031 0.34563
H*11 H 0.38950 -0.08055 0.32471
H*12 H 0.29439 -0.21849 0.33203
C1+ C 0.11861 0.19589 0.60720
N'2+ N -0.01475 0.32280 0.55886
N3+ N 0.02019 0.21076 0.52659
N'4+ N 0.10360 0.12833 0.55597
N'5+ N 0.04788 0.31166 0.61003
C6+ C 0.19900 0.13973 0.65563
N7+ N 0.17655 0.21540 0.71317
O8+ O 0.12703 0.15249 0.75273
O9+ O 0.21236 0.33466 0.71374
N10+ N 0.16991 -0.01747 0.66413
O11+ O 0.05593 -0.04672 0.66814
O12+ O 0.26235 -0.09628 0.66511
N13+ N 0.35204 0.14614 0.64821
O14+ O 0.38918 0.15408 0.59873
O15+ O 0.41910 0.14353 0.69328
O16+ O -0.02218 0.18964 0.47535

#END

data_FTNM_2O_AGH_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.851
_cell_length_b                 10.180
```

```
_cell_length_c                 24.888
_cell_angle_alpha               90.00
_cell_angle_beta               109.50
_cell_angle_gamma               90.00
_cell_volume                  2352.69
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.25782 0.51177 0.93913
N2 N -0.21411 0.53213 0.99553
H*3 H -0.14639 0.60638 1.01382
H*4 H -0.24777 0.47363 1.02136
N5 N -0.21044 0.59200 0.90618
H*6 H -0.14240 0.66676 0.92429
N7 N -0.34694 0.41404 0.91509
H*8 H -0.38475 0.35186 0.93839
H*9 H -0.37665 0.40301 0.87222
N10 N -0.25647 0.57025 0.84729
H*11 H -0.31134 0.64993 0.82613
H*12 H -0.17056 0.55079 0.83448
C1+ C 0.14429 -0.14182 0.10376
N'2+ N -0.02184 -0.27105 0.05627
N3+ N 0.06075 -0.23135 0.02447
N'4+ N 0.16693 -0.15040 0.05333
N'5+ N 0.03287 -0.21405 0.10660
C6+ C 0.24092 -0.06636 0.15132
N7+ N 0.21564 -0.09638 0.20767
O8+ O 0.31108 -0.15091 0.24552
O9+ O 0.09906 -0.06086 0.20914
N10+ N 0.40252 -0.09605 0.15854
O11+ O 0.43445 -0.21142 0.16141
O12+ O 0.48093 -0.00254 0.15979
N13+ N 0.22858 0.08894 0.14530
O14+ O 0.17864 0.13242 0.09738
O15+ O 0.26971 0.15110 0.18976
O16+ O 0.03770 -0.26774 -0.02594

#END

data_FTNM_2O_AGH_5
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 10.983
```

_cell_length_b 7.786
_cell_length_c 6.927
_cell_angle_alpha 96.45
_cell_angle_beta 83.29
_cell_angle_gamma 82.75
_cell_volume 578.717
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.16747 0.23320 0.70141
N2 N -0.04383 0.22173 0.66995
H*3 H 0.00078 0.23709 0.53830
H*4 H 0.00828 0.19736 0.77729
N5 N -0.23357 0.26588 0.55442
H*6 H -0.18933 0.28144 0.42184
N7 N -0.22609 0.21297 0.87471
H*8 H -0.17972 0.18832 0.98842
H*9 H -0.31979 0.22294 0.89065
N10 N -0.36269 0.27771 0.58817
H*11 H -0.40282 0.39854 0.56812
H*12 H -0.39223 0.18423 0.49707
C1+ C 0.19826 0.25566 0.03912
N'2+ N 0.08948 0.25212 0.31288
N3+ N 0.02630 0.20505 0.16030
N'4+ N 0.09267 0.20503 -0.01426
N'5+ N 0.19872 0.28296 0.23385
C6+ C 0.30379 0.26696 -0.10680
N7+ N 0.42218 0.28488 -0.01296
O8+ O 0.50841 0.16608 -0.05182
O9+ O 0.41835 0.42112 0.09380
N10+ N 0.32854 0.10133 -0.26538
O11+ O 0.33762 -0.03755 -0.20115
O12+ O 0.33465 0.12519 -0.43707
N13+ N 0.28874 0.42640 -0.23059
O14+ O 0.18383 0.49052 -0.24229
O15+ O 0.38472 0.47139 -0.30219
O16+ O -0.08154 0.16686 0.18442

#END

S32. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidinium 5-(trinitromethyl)tetrazolate 2*N*-oxide (ionic form).
data_FTNM_2O_DAGH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 18.473
_cell_length_b                 6.702
_cell_length_c                 9.687
_cell_angle_alpha               90.00
_cell_angle_beta                92.74
_cell_angle_gamma                 90.00
_cell_volume                   1197.94
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.58432 -0.31319 0.30678
N2 N 0.59132 -0.29763 0.17027
H*3 H 0.61802 -0.40877 0.12254
N4 N 0.61255 -0.47323 0.37422
H*5 H 0.60752 -0.48631 0.47764
N6 N 0.54986 -0.17199 0.37481
H*7 H 0.52949 -0.05427 0.31987
H*8 H 0.54381 -0.17998 0.47767
N9 N 0.64842 -0.61875 0.29946
N10 N 0.56186 -0.13090 0.10071
H*11 H 0.52396 -0.17551 0.02734
H*12 H 0.70102 -0.63054 0.33496
H*13 H 0.62295 -0.75277 0.30675
H*14 H 0.60185 -0.05357 0.05548
C1+ C 0.11883 0.06198 -0.23262
N'2+ N 0.03991 -0.12411 -0.14526
N3+ N 0.04693 -0.16842 -0.28221
N'4+ N 0.09658 -0.05446 -0.34004
N'5+ N 0.08614 0.02163 -0.11497
C6+ C 0.17699 0.20839 -0.24519
N7+ N 0.20499 0.28732 -0.10379
O8+ O 0.26703 0.24800 -0.06414
O9+ O 0.16108 0.38573 -0.04353
N10+ N 0.24203 0.11479 -0.32142
O11+ O 0.26443 -0.04236 -0.27462
O12+ O 0.26366 0.20444 -0.42099
N13+ N 0.15656 0.40278 -0.33246
O14+ O 0.10558 0.38932 -0.41546
O15+ O 0.19387 0.54985 -0.30736
O16+ O 0.01043 -0.30122 -0.34458

#END

data_FTNM_2O_DAGH_2
_symmetry_cell_setting          monoclinic
```

```
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   12.879
_cell_length_b                   10.534
_cell_length_c                   10.219
_cell_angle_alpha                 90.00
_cell_angle_beta                  116.48
_cell_angle_gamma                    90.00
_cell_volume                     1240.94
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.52911 0.70271 0.27477
N2 N 0.60326 0.77681 0.38227
H*3 H 0.67647 0.80523 0.37632
N4 N 0.55427 0.66938 0.16477
H*5 H 0.49862 0.61327 0.08286
N6 N 0.43173 0.66258 0.27682
H*7 H 0.41636 0.69001 0.36170
H*8 H 0.37435 0.60666 0.19721
N9 N 0.65737 0.71327 0.16613
N10 N 0.57662 0.81116 0.49635
H*11 H 0.57037 0.90734 0.49995
H*12 H 0.70898 0.63882 0.16974
H*13 H 0.63967 0.76752 0.07618
H*14 H 0.63951 0.77894 0.59330
C1+ C -0.05135 0.38473 0.20412
N'2+ N -0.17345 0.51947 0.20598
N3+ N -0.21847 0.45170 0.07794
N'4+ N -0.14385 0.36547 0.07375
N'5+ N -0.06758 0.47551 0.28537
C6+ C 0.05288 0.30587 0.25255
N7+ N 0.13390 0.32379 0.41583
O8+ O 0.14901 0.23443 0.49833
O9+ O 0.17705 0.42887 0.44772
N10+ N 0.01944 0.16172 0.22273
O11+ O -0.04647 0.12328 0.26912
O12+ O 0.06029 0.10162 0.15466
N13+ N 0.13261 0.33088 0.17319
O14+ O 0.08650 0.37972 0.05333
O15+ O 0.23407 0.29940 0.24079
O16+ O -0.31849 0.46986 -0.02278
```

```
#END

data_FTNM_2O_DAGH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 10.878
_cell_length_b                 11.590
_cell_length_c                 9.579
_cell_angle_alpha               90.00
_cell_angle_beta                75.60
_cell_angle_gamma                90.00
_cell_volume                   1169.74
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.76256 -0.37556 0.19462
N2 N 0.74668 -0.35072 0.33448
H*3 H 0.66875 -0.30419 0.38378
N4 N 0.67581 -0.33836 0.12603
H*5 H 0.68703 -0.35675 0.02007
N6 N 0.86296 -0.43630 0.12441
H*7 H 0.92577 -0.46250 0.18033
H*8 H 0.87724 -0.45622 0.01902
N9 N 0.57146 -0.27473 0.20315
N10 N 0.83720 -0.38964 0.40523
H*11 H 0.79534 -0.44283 0.48805
H*12 H 0.57122 -0.19474 0.15931
H*13 H 0.48918 -0.31675 0.20360
H*14 H 0.87719 -0.32110 0.44386
C1+ C 0.36116 0.43117 0.24542
N'2+ N 0.23607 0.57306 0.30898
N3+ N 0.20267 0.50989 0.20303
N'4+ N 0.27926 0.41945 0.16122
N'5+ N 0.33638 0.52177 0.33538
C6+ C 0.46163 0.34641 0.24239
N7+ N 0.52220 0.36143 0.36987
O8+ O 0.50808 0.28504 0.46009
O9+ O 0.58097 0.45095 0.36772
N10+ N 0.40820 0.22033 0.24476
O11+ O 0.31413 0.20062 0.34007
```

O12+ O 0.46344 0.15412 0.15103
N13+ N 0.57768 0.34915 0.10376
O14+ O 0.55796 0.39152 -0.00430
O15+ O 0.67732 0.30890 0.11868
O16+ O 0.11045 0.53536 0.15223

#END

data_FTNM_2O_DAGH_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 11.462
_cell_length_b 11.346
_cell_length_c 9.244
_cell_angle_alpha 90.00
_cell_angle_beta 100.75
_cell_angle_gamma 90.00
_cell_volume 1181.06
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.43374 0.43367 0.83220
N2 N 0.53451 0.37984 0.81625
H*3 H 0.58872 0.42277 0.75839
N4 N 0.40875 0.54096 0.77173
H*5 H 0.33262 0.58243 0.78323
N6 N 0.35926 0.38160 0.90696
H*7 H 0.38168 0.30090 0.95054
H*8 H 0.28273 0.42019 0.92064
N9 N 0.48902 0.59307 0.69390
N10 N 0.56001 0.26830 0.87937
H*11 H 0.63744 0.27131 0.95406
H*12 H 0.44939 0.60727 0.58730
H*13 H 0.52000 0.67039 0.74228
H*14 H 0.56699 0.20834 0.79944
C1+ C 0.52314 0.07422 0.26060
N'2+ N 0.36325 -0.00170 0.14478
N3+ N 0.36944 0.11568 0.11153
N'4+ N 0.46952 0.16591 0.18215
N'5+ N 0.46166 -0.02698 0.23889
C6+ C 0.64136 0.08589 0.35235

```
N7+ N 0.69606 -0.03436 0.40160
O8+ O 0.78433 -0.06594 0.35605
O9+ O 0.64448 -0.08784 0.48480
N10+ N 0.72715 0.15365 0.26718
O11+ O 0.73152 0.11544 0.14590
O12+ O 0.78013 0.23875 0.32776
N13+ N 0.64804 0.15847 0.50066
O14+ O 0.56827 0.22773 0.50498
O15+ O 0.73295 0.13731 0.59815
O16+ O 0.28942 0.16857 0.02454

#END

data_FTNM_2O_DAGH_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 13.409
_cell_length_b                 14.442
_cell_length_c                 6.995
_cell_angle_alpha               90.00
_cell_angle_beta                115.30
_cell_angle_gamma               90.00
_cell_volume                   1224.67
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.20822 -0.64734 0.49655
N2 N -0.27110 -0.61873 0.59087
H*3 H -0.23708 -0.57369 0.71361
N4 N -0.10396 -0.61570 0.56726
H*5 H -0.05570 -0.63700 0.49680
N6 N -0.24843 -0.70637 0.33483
H*7 H -0.32728 -0.72834 0.28698
H*8 H -0.20284 -0.72905 0.26090
N9 N -0.06440 -0.55374 0.73754
N10 N -0.37943 -0.65186 0.51665
H*11 H -0.43354 -0.59800 0.46626
H*12 H 0.00154 -0.58148 0.86117
H*13 H -0.04292 -0.49263 0.69285
H*14 H -0.38918 -0.68663 0.63419
C1+ C 0.60304 -0.31206 0.00239
```

N'2+ N 0.47864 -0.21269 -0.03864
N3+ N 0.52741 -0.19492 -0.17178
N'4+ N 0.60575 -0.25666 -0.15061
N'5+ N 0.52702 -0.28751 0.07015
C6+ C 0.67304 -0.39442 0.07367
N7+ N 0.63727 -0.45827 0.20845
O8+ O 0.60092 -0.53472 0.13953
O9+ O 0.64976 -0.42528 0.37719
N10+ N 0.67068 -0.45062 -0.12047
O11+ O 0.57950 -0.46889 -0.25533
O12+ O 0.75903 -0.46980 -0.12154
N13+ N 0.80043 -0.37587 0.21521
O14+ O 0.83547 -0.30043 0.19837
O15+ O 0.85191 -0.43934 0.33029
O16+ O 0.50060 -0.12796 -0.29803

#END

S33. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidinium 5-(trinitromethyl)tetrazolate 2*N*-oxide (ionic form).

data_FTNM_2O_TAGH_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 10.567
_cell_length_b 8.198
_cell_length_c 9.296
_cell_angle_alpha 116.87
_cell_angle_beta 110.85
_cell_angle_gamma 84.24
_cell_volume 669.541
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.88095 0.08770 -0.29041
N2 N 0.83677 -0.08845 -0.36017
H*3 H 0.73493 -0.12036 -0.41835
N4 N 1.01429 0.13718 -0.21213
H*5 H 1.07856 0.03705 -0.20840
N6 N 0.79179 0.21437 -0.29893
H*7 H 0.82936 0.34640 -0.24448
N8 N 1.05786 0.32217 -0.14023
N9 N 0.93202 -0.21821 -0.34955
H*10 H 0.92546 -0.31437 -0.46995

H*11 H 1.10889 0.37067 -0.01133
H*12 H 1.11967 0.33629 -0.19720
H*13 H 0.91468 -0.27998 -0.28407
N14 N 0.65297 0.15914 -0.38145
H*15 H 0.60311 0.22399 -0.29702
H*16 H 0.61389 0.18960 -0.48289
C1+ C 0.50328 0.33333 0.24637
N'2+ N 0.37282 0.29298 0.35826
N3+ N 0.30568 0.36510 0.24636
N'4+ N 0.38495 0.39115 0.17295
N'5+ N 0.49791 0.27259 0.35630
C6+ C 0.62193 0.32812 0.19829
N7+ N 0.73236 0.21732 0.26525
O8+ O 0.75914 0.07494 0.16097
O9+ O 0.78461 0.28551 0.42122
N10+ N 0.58007 0.24290 -0.00265
O11+ O 0.51470 0.09625 -0.08275
O12+ O 0.61424 0.33069 -0.06103
N13+ N 0.69756 0.52105 0.26718
O14+ O 0.63163 0.65393 0.30360
O15+ O 0.81638 0.51860 0.27865
O16+ O 0.18371 0.40179 0.21774

#END

data_FTNM_2O_TAGH_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 18.580
_cell_length_b 9.093
_cell_length_c 8.303
_cell_angle_alpha 90.00
_cell_angle_beta 116.75
_cell_angle_gamma 90.00
_cell_volume 1252.65
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.69980 0.02709 0.34871
N2 N 0.64933 -0.05633 0.21097
H*3 H 0.59365 -0.07596 0.20126

N4 N 0.77394 0.05634 0.36777
H*5 H 0.78958 0.01323 0.27497
N6 N 0.67613 0.08126 0.46739
H*7 H 0.71617 0.14400 0.56990
N8 N 0.82555 0.14382 0.51287
N9 N 0.67552 -0.11163 0.08877
H*10 H 0.63931 -0.07370 -0.03761
H*11 H 0.87608 0.08603 0.59283
H*12 H 0.84113 0.23593 0.46612
H*13 H 0.67427 -0.22360 0.08910
N14 N 0.59833 0.04909 0.44449
H*15 H 0.60148 -0.00601 0.55427
H*16 H 0.56653 0.14389 0.42756
C1+ C 0.06472 0.00811 0.78964
N'2+ N -0.01407 -0.16407 0.63851
N3+ N 0.06495 -0.20559 0.70114
N'4+ N 0.11612 -0.09974 0.79782
N'5+ N -0.01333 -0.02851 0.69650
C6+ C 0.09389 0.14738 0.88570
N7+ N 0.02566 0.23738 0.89358
O8+ O 0.02693 0.25781 1.04005
O9+ O -0.02444 0.28169 0.74785
N10+ N 0.16089 0.11911 1.08318
O11+ O 0.14305 0.03205 1.16979
O12+ O 0.22474 0.18406 1.13176
N13+ N 0.13510 0.25668 0.80269
O14+ O 0.16214 0.20259 0.70795
O15+ O 0.13537 0.38640 0.84076
O16+ O 0.08580 -0.32928 0.66987

#END

data_FTNM_2O_TAGH_3
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 9.664
_cell_length_b 8.978
_cell_length_c 9.309
_cell_angle_alpha 98.59
_cell_angle_beta 105.88
_cell_angle_gamma 54.63
_cell_volume 633.431
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x

```
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25903 -0.12609 0.27631
N2 N 0.23349 -0.15085 0.12819
H*3 H 0.13254 -0.04210 0.06193
N4 N 0.39033 -0.26505 0.36873
H*5 H 0.46757 -0.38698 0.32209
N6 N 0.15327 0.03763 0.33201
H*7 H 0.17698 0.05081 0.44490
N8 N 0.41427 -0.23565 0.52310
N9 N 0.34584 -0.32328 0.07277
H*10 H 0.40818 -0.31354 0.00613
H*11 H 0.40293 -0.32016 0.57338
H*12 H 0.53437 -0.25953 0.56628
H*13 H 0.27674 -0.37417 0.01322
N14 N 0.01698 0.18066 0.23306
H*15 H -0.09974 0.22512 0.25297
H*16 H 0.03170 0.28575 0.24588
C1+ C 0.04384 0.33335 0.68554
N'2+ N -0.19775 0.56468 0.57642
N3+ N -0.16913 0.40640 0.50705
N'4+ N -0.01836 0.25805 0.57371
N'5+ N -0.06202 0.51622 0.68999
C6+ C 0.20718 0.22015 0.79571
N7+ N 0.22993 0.33108 0.93110
O8+ O 0.22868 0.29678 1.05252
O9+ O 0.24860 0.44559 0.90299
N10+ N 0.21482 0.05820 0.85129
O11+ O 0.08873 0.10188 0.89451
O12+ O 0.34333 -0.09587 0.84453
N13+ N 0.38103 0.12302 0.73834
O14+ O 0.36760 0.10047 0.60486
O15+ O 0.51334 0.08068 0.83419
O16+ O -0.27388 0.40362 0.39388

#END

data_FTNM_2O_TAGH_4
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 13.397
_cell_length_b                 10.149
_cell_length_c                 9.850
_cell_angle_alpha               90.00
```

```
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
_cell_volume                   1339.27
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.40449 -0.10575 0.38640
N2 N 0.32083 -0.07295 0.31979
H*3 H 0.32643 -0.00437 0.24496
N4 N 0.40124 -0.19569 0.48599
H*5 H 0.33393 -0.23672 0.50792
N6 N 0.49139 -0.04861 0.35342
H*7 H 0.55311 -0.07617 0.40632
N8 N 0.48972 -0.22826 0.55406
N9 N 0.23095 -0.13409 0.35620
H*10 H 0.20258 -0.18407 0.27526
H*11 H 0.48298 -0.20707 0.65471
H*12 H 0.50472 -0.32594 0.54205
H*13 H 0.18084 -0.06520 0.38792
N14 N 0.49280 0.04510 0.24894
H*15 H 0.51704 0.13332 0.28556
H*16 H 0.53878 0.01446 0.17290
C1+ C 0.15413 0.65746 0.02537
N'2+ N 0.04142 0.66988 0.17663
N3+ N 0.02243 0.56828 0.08850
N'4+ N 0.09244 0.55738 -0.00759
N'5+ N 0.12551 0.72517 0.13580
C6+ C 0.24669 0.68124 -0.04981
N7+ N 0.31582 0.77771 0.02477
O8+ O 0.39554 0.73708 0.06756
O9+ O 0.28330 0.88927 0.03342
N10+ N 0.30424 0.54853 -0.07436
O11+ O 0.31812 0.48212 0.02612
O12+ O 0.32857 0.52243 -0.19063
N13+ N 0.23413 0.74219 -0.19740
O14+ O 0.15421 0.72564 -0.25248
O15+ O 0.30623 0.80151 -0.24217
O16+ O -0.05255 0.49490 0.09834

#END

data_FTNM_2O_TAGH_5
_symmetry_cell_setting           monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 8.752
_cell_length_b 18.026
_cell_length_c 9.102
_cell_angle_alpha 90.00
_cell_angle_beta 109.98
_cell_angle_gamma 90.00
_cell_volume 1349.54
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.05709 0.37215 0.87344
N2 N -0.03004 0.32300 0.99014
H*3 H -0.11991 0.31518 1.03570
N4 N 0.05744 0.38456 0.80918
H*5 H 0.16308 0.35560 0.85224
N6 N -0.19866 0.40889 0.82100
H*7 H -0.21444 0.44567 0.73237
N8 N 0.02619 0.43620 0.68736
N9 N 0.11893 0.28533 1.04284
H*10 H 0.09984 0.22966 1.02829
H*11 H 0.10957 0.47792 0.71879
H*12 H 0.03128 0.41084 0.58916
H*13 H 0.17813 0.29675 1.15792
N14 N -0.31639 0.39492 0.89012
H*15 H -0.34154 0.44241 0.93805
H*16 H -0.41982 0.37532 0.80843
C1+ C 0.46489 0.12756 0.86014
N'2+ N 0.42274 0.09506 1.06745
N3+ N 0.28635 0.12687 0.96303
N'4+ N 0.30871 0.14756 0.83077
N'5+ N 0.53482 0.09550 1.00029
C6+ C 0.54316 0.13649 0.74244
N7+ N 0.70458 0.09402 0.78627
O8+ O 0.71474 0.04191 0.70457
O9+ O 0.81040 0.11767 0.90175
N10+ N 0.42787 0.10894 0.57828
O11+ O 0.37284 0.04713 0.57653
O12+ O 0.40148 0.15154 0.46825
N13+ N 0.58778 0.21911 0.71157
O14+ O 0.51166 0.26824 0.74600
O15+ O 0.69625 0.22589 0.65668
O16+ O 0.15637 0.13522 0.99045

#END

S34. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 5-nitrotetrazole (cocrystal form).

```
data_T_NH3_1
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.665
_cell_length_b                 12.005
_cell_length_c                 9.601
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1113.99
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.25501 0.84525 -0.92367
H*2 H 0.18719 0.88165 -0.99101
H*3 H 0.35196 0.86476 -0.95751
H*4 H 0.24220 0.88342 -0.82974
C1+ C -0.14488 0.11269 0.41005
N'2+ N -0.20782 0.11018 0.28425
N'3+ N -0.10761 0.11339 0.19297
N4+ N 0.00922 0.11762 0.26715
N'5+ N -0.00790 0.11739 0.40355
N6+ N -0.22018 0.11044 0.54232
O7+ O -0.34628 0.10608 0.53482
O8+ O -0.15036 0.11313 0.64855
H*9+ H 0.10400 0.12076 0.22176

#END

data_T_NH3_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
```

```
_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
_cell_length_a                 9.661
_cell_length_b                 9.582
_cell_length_c                 6.130
_cell_angle_alpha               90.00
_cell_angle_beta                88.83
_cell_angle_gamma                 90.00
_cell_volume                   567.346
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.27603 0.57480 0.31059
H*2 H -0.36866 0.54177 0.25301
H*3 H -0.20288 0.50638 0.25424
H*4 H -0.25520 0.66852 0.23851
C1+ C 0.33905 0.41150 0.22130
N'2+ N 0.27439 0.28631 0.21921
N'3+ N 0.37345 0.19351 0.22171
N4+ N 0.49137 0.26626 0.22513
N'5+ N 0.47606 0.40315 0.22505
N6+ N 0.26546 0.54504 0.21960
O7+ O 0.13916 0.53923 0.21611
O8+ O 0.33675 0.65053 0.22182
H*9+ H 0.58562 0.21950 0.22761

#END

data_T_NH3_3
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 6.057
_cell_length_b                 9.582
_cell_length_c                 9.656
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   560.417
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.80836 0.32787 0.73529
H*2 H 0.75352 0.25963 0.80857
H*3 H 0.75170 0.29274 0.64223
H*4 H 0.73198 0.42077 0.75383
C1+ C 0.77030 0.15911 0.35157
N'2+ N 0.78097 0.03371 0.28759
N'3+ N 0.76701 -0.05876 0.38667
N4+ N 0.74885 0.01438 0.50391
N'5+ N 0.74997 0.15121 0.48814
N6+ N 0.78013 0.29239 0.27774
O7+ O 0.79897 0.28617 0.15189
O8+ O 0.76863 0.39811 0.34839
H*9+ H 0.73521 -0.03207 0.59801

#END

data_T_NH3_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 5.661
_cell_length_b                 9.664
_cell_length_c                 11.390
_cell_angle_alpha               90.00
_cell_angle_beta               117.09
_cell_angle_gamma                90.00
_cell_volume                   554.762
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.59692 0.74126 -0.11762
H*2 H 0.74186 0.81341 -0.09681
H*3 H 0.67129 0.64923 -0.12950
H*4 H 0.56918 0.73201 -0.03563
C1+ C 0.12745 0.63310 0.16022
N'2+ N -0.01308 0.69515 0.21481
```

```
N'3+ N -0.08049 0.59566 0.27129
N4+ N 0.02126 0.48010 0.24831
N'5+ N 0.15341 0.49738 0.17925
N6+ N 0.24170 0.70801 0.08646
O7+ O 0.20434 0.83291 0.07556
O8+ O 0.36431 0.63909 0.04228
H*9+ H -0.00162 0.38609 0.28160

#END

data_T_NH3_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 6.130
_cell_length_b                 9.563
_cell_length_c                 9.668
_cell_angle_alpha               90.00
_cell_angle_beta                95.69
_cell_angle_gamma                 90.00
_cell_volume                   563.957
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.68764 0.42250 0.27253
H*2 H 0.73199 0.49144 0.19997
H*3 H 0.76184 0.32983 0.25446
H*4 H 0.75510 0.45751 0.36676
C1+ C 0.22481 0.41010 0.33975
N'2+ N 0.22926 0.28464 0.27548
N'3+ N 0.23621 0.19181 0.37500
N4+ N 0.23562 0.26481 0.49278
N'5+ N 0.22862 0.40189 0.47695
N6+ N 0.21653 0.54375 0.26559
O7+ O 0.21367 0.53778 0.13916
O8+ O 0.21320 0.64948 0.33658
H*9+ H 0.24023 0.21810 0.58731

#END
```

S35. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 5-nitrotetrazole (cocrystal form).

```
data_T_NH2OH_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21'
_symmetry_Int_Tables_number      4
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,-z
_cell_length_a                   7.891
_cell_length_b                   5.114
_cell_length_c                   6.916
_cell_angle_alpha                 90.00
_cell_angle_beta                  93.85
_cell_angle_gamma                    90.00
_cell_volume                     278.462
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.51564 0.65302 0.13684
H*2 H 0.59282 0.81278 0.12976
H*3 H 0.59329 0.49425 0.12705
O4 O 0.41644 0.65545 -0.04665
H*5 H 0.30130 0.65429 -0.00761
C1+ C -0.12872 0.82220 0.68283
N'2+ N -0.18584 0.99842 0.54789
N'3+ N -0.33971 0.92285 0.49258
N4+ N -0.36747 0.70775 0.59543
N'5+ N -0.23976 0.63572 0.71681
N6+ N 0.04037 0.83421 0.78339
O7+ O 0.13128 1.01536 0.73962
O8+ O 0.07575 0.66215 0.90220
H*9+ H -0.47864 0.60747 0.58105

#END

data_T_NH2OH_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   11.580
_cell_length_b                   9.653
```

```
_cell_length_c                  5.120
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                  90.00
_cell_volume                    572.323
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.17723 0.05168 0.24660
H*2 H -0.20709 0.10683 0.40307
H*3 H -0.20570 0.10359 0.08495
O4 O -0.24596 -0.07333 0.24959
H*5 H -0.18811 -0.14527 0.25349
C1+ C 0.57751 0.37536 -0.00605
N'2+ N 0.51037 0.42237 0.19115
N'3+ N 0.48012 0.31211 0.32247
N4+ N 0.52981 0.20550 0.19977
N'5+ N 0.59180 0.23901 -0.00716
N6+ N 0.63020 0.46594 -0.20199
O7+ O 0.61071 0.58983 -0.18038
O8+ O 0.68901 0.40975 -0.36984
H*9+ H 0.52046 0.10619 0.26146

#END

data_T_NH2OH_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21'
_symmetry_Int_Tables_number      4
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,-z
_cell_length_a                  7.979
_cell_length_b                  5.166
_cell_length_c                  8.629
_cell_angle_alpha                90.00
_cell_angle_beta                 55.58
_cell_angle_gamma                  90.00
_cell_volume                    293.409
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.51339 0.26296 0.10444
H*2 H 0.60530 0.42143 0.04561
```

H*3 H 0.60730 0.10612 0.04621
O4 O 0.39880 0.25970 0.02142
H*5 H 0.26001 0.25879 0.13002
C1+ C 0.14647 -0.19998 0.70988
N'2+ N 0.01004 -0.33887 0.69854
N'3+ N 0.11593 -0.51857 0.57368
N4+ N 0.30835 -0.47980 0.51662
N'5+ N 0.33639 -0.28304 0.59716
N6+ N 0.09122 0.02259 0.83492
O7+ O -0.08876 0.08052 0.93208
O8+ O 0.22985 0.13085 0.83116
H*9+ H 0.42415 -0.59349 0.41858

#END

data_T_NH2OH_4
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P n a 21'
_symmetry_Int_Tables_number 33
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 13.175
_cell_length_b 8.207
_cell_length_c 5.076
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 548.854
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.06497 0.44640 0.57520
H*2 H -0.04231 0.38061 0.73574
H*3 H -0.04172 0.38098 0.41483
O4 O 0.00141 0.58665 0.57645
H*5 H -0.04581 0.67656 0.57614
C1+ C 0.34917 0.47243 0.09867
N'2+ N 0.28339 0.44861 0.29961
N'3+ N 0.24388 0.30481 0.25838
N4+ N 0.28716 0.24970 0.03767
N'5+ N 0.35367 0.34955 -0.07075
N6+ N 0.41036 0.62017 0.06878
O7+ O 0.39954 0.72488 0.23763
O8+ O 0.46684 0.62581 -0.12227

H*9+ H 0.27005 0.13920 -0.04046

#END

data_T_NH2OH_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21'
_symmetry_Int_Tables_number 4
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,-z
_cell_length_a 6.975
_cell_length_b 5.080
_cell_length_c 8.703
_cell_angle_alpha 90.00
_cell_angle_beta 112.54
_cell_angle_gamma 90.00
_cell_volume 284.817
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.11555 0.45511 -0.53582
H*2 H 0.05297 0.61806 -0.60606
H*3 H 0.04762 0.29745 -0.60958
O4 O 0.02559 0.45492 -0.41129
H*5 H 0.14633 0.45055 -0.30860
C1+ C 0.30530 0.03472 0.11314
N'2+ N 0.26172 -0.13993 0.21255
N'3+ N 0.35464 -0.04897 0.36355
N4+ N 0.44840 0.17298 0.34803
N'5+ N 0.42278 0.23497 0.19409
N6+ N 0.23034 0.00725 -0.06787
O7+ O 0.12328 -0.18575 -0.12810
O8+ O 0.28138 0.17961 -0.14280
H*9+ H 0.53299 0.28530 0.44742

#END

S36. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 5-nitrotetrazole (cocrystal form).
data_T_N2H4_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.560
_cell_length_b                 10.483
_cell_length_c                 6.398
_cell_angle_alpha               90.00
_cell_angle_beta                95.77
_cell_angle_gamma                 90.00
_cell_volume                   637.943
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.19783 0.03064 0.33508
H*2 H 0.19663 0.06042 0.48668
H*3 H 0.12194 -0.03690 0.30697
N4 N 0.32972 -0.02675 0.29893
H*5 H 0.39373 0.04377 0.25518
H*6 H 0.37787 -0.06830 0.43131
C1+ C 0.34292 0.74977 -0.02213
N'2+ N 0.25262 0.69123 0.08602
N'3+ N 0.33267 0.63381 0.24640
N'4+ N 0.46614 0.65631 0.23666
N5+ N 0.47454 0.72977 0.06716
N6+ N 0.31417 0.82637 -0.21096
O7+ O 0.19230 0.83996 -0.28207
O8+ O 0.41913 0.87094 -0.28162
H*9+ H 0.56691 0.76182 0.02178

#END

data_T_N2H4_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P c a 21'
_symmetry_Int_Tables_number      29
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.507
_cell_length_b                 6.195
_cell_length_c                 11.144
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
```

```
_cell_volume                    656.336
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.93160 -0.21723 0.45962
H*2 H 0.89796 -0.08209 0.41589
H*3 H 0.85807 -0.25572 0.52232
N4 N 1.06237 -0.18209 0.52120
H*5 H 1.14143 -0.21750 0.46299
H*6 H 1.07419 -0.02523 0.54718
C1+ C 0.08951 0.52446 -0.25538
N'2+ N -0.00131 0.38768 -0.30092
N'3+ N 0.07730 0.25091 -0.36846
N'4+ N 0.21043 0.30192 -0.36437
N5+ N 0.22006 0.47517 -0.29299
N6+ N 0.06224 0.70571 -0.17586
O7+ O -0.05872 0.73969 -0.14591
O8+ O 0.16740 0.80926 -0.14611
H*9+ H 0.31247 0.54938 -0.27389

#END

data_T_N2H4_3
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  5.984
_cell_length_b                  10.854
_cell_length_c                  9.131
_cell_angle_alpha                 90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                    593.062
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.83532 0.46707 -0.55774
H*2 H 0.75036 0.43548 -0.46845
H*3 H 0.98120 0.50450 -0.52195
```

N4 N 0.71424 0.56182 -0.63373
H*5 H 0.61546 0.51999 -0.70948
H*6 H 0.61308 0.61073 -0.56512
C1+ C -0.40517 0.19712 0.77007
N'2+ N -0.41725 0.14579 0.89991
N'3+ N -0.22579 0.07952 0.91253
N'4+ N -0.10206 0.08992 0.79544
N5+ N -0.21340 0.16423 0.70391
N6+ N -0.56651 0.27816 0.70015
O7+ O -0.73591 0.30356 0.76717
O8+ O -0.51364 0.31381 0.57667
H*9+ H -0.15503 0.18828 0.60363

#END

data_T_N2H4_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 9.511
_cell_length_b 12.420
_cell_length_c 6.481
_cell_angle_alpha 90.00
_cell_angle_beta 60.89
_cell_angle_gamma 90.00
_cell_volume 668.876
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.35047 -0.39759 0.91441
H*2 H 0.39423 -0.47049 0.83726
H*3 H 0.39719 -0.38116 1.02259
N4 N 0.17826 -0.39832 1.05690
H*5 H 0.13134 -0.37745 0.95113
H*6 H 0.13527 -0.47279 1.12453
C1+ C -0.00096 0.25828 0.51471
N'2+ N -0.11797 0.18738 0.59805
N'3+ N -0.08431 0.12083 0.73447
N'4+ N 0.04760 0.14982 0.73448
N5+ N 0.10207 0.23692 0.59588
N6+ N 0.02282 0.34845 0.35801
O7+ O -0.07574 0.36238 0.29235

```
O8+ O 0.14377 0.40306 0.30632
H*9+ H 0.20392 0.27650 0.56417

#END

data_T_N2H4_5
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.453
_cell_length_b                 12.464
_cell_length_c                 10.581
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1246.68
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.18119 0.32439 0.46856
H*2 H -0.18181 0.24589 0.44130
H*3 H -0.09783 0.33510 0.52797
N4 N -0.30734 0.35310 0.53631
H*5 H -0.37984 0.37840 0.47188
H*6 H -0.34965 0.28932 0.58344
C1+ C -0.16331 0.01163 0.75489
N'2+ N -0.26267 -0.04035 0.81608
N'3+ N -0.19381 -0.12084 0.87680
N'4+ N -0.05822 -0.11817 0.85370
N5+ N -0.03702 -0.03458 0.77648
N6+ N -0.17821 0.10535 0.67421
O7+ O -0.29600 0.14242 0.65940
O8+ O -0.06684 0.13857 0.62778
H*9+ H 0.05971 -0.01365 0.74316

#END
```

S37. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 5-nitrotetrazole (cocrystal form).

```
data_T_G_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.743
_cell_length_b                 11.039
_cell_length_c                 8.695
_cell_angle_alpha               90.00
_cell_angle_beta                134.27
_cell_angle_gamma               90.00
_cell_volume                   669.639
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.11088 0.24914 0.27300
N'2 N -0.00100 0.27973 0.29622
H*3 H -0.02042 0.37131 0.28462
N4 N 0.17288 0.12962 0.30703
H*5 H 0.17755 0.09780 0.20139
H*6 H 0.10347 0.07330 0.32599
N7 N 0.18269 0.32378 0.21261
H*8 H 0.16197 0.41337 0.21433
H*9 H 0.31771 0.30412 0.28304
C1+ C 0.08503 0.27091 0.77091
N'2+ N -0.02665 0.19468 0.75683
N'3+ N 0.02163 0.08405 0.73850
N'4+ N 0.15697 0.09232 0.74125
N5+ N 0.19892 0.21028 0.76173
N6+ N 0.09365 0.40190 0.79327
O7+ O -0.01408 0.44999 0.80038
O8+ O 0.21256 0.45221 0.80301
H*9+ H 0.30022 0.24288 0.76827

#END

data_T_G_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
```

```
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.433
_cell_length_b                 11.125
_cell_length_c                 9.726
_cell_angle_alpha               90.00
_cell_angle_beta                56.11
_cell_angle_gamma                 90.00
_cell_volume                   667.627
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.22905 0.24882 0.15594
N'2 N 0.20090 0.21931 0.29438
H*3 H 0.20155 0.12821 0.30625
N4 N 0.20940 0.36845 0.12348
H*5 H 0.32017 0.39606 0.00608
H*6 H 0.19632 0.42487 0.21041
N7 N 0.28191 0.17272 0.02392
H*8 H 0.26929 0.08408 0.05101
H*9 H 0.21415 0.19489 -0.03873
C1+ C 0.73406 0.27080 0.19645
N'2+ N 0.73888 0.19497 0.29764
N'3+ N 0.74098 0.08461 0.23719
N'4+ N 0.73758 0.09267 0.10477
N5+ N 0.73317 0.21021 0.07716
N6+ N 0.73004 0.40138 0.20319
O7+ O 0.73115 0.44947 0.31496
O8+ O 0.72579 0.45138 0.09186
H*9+ H 0.72985 0.24256 -0.01888

#END

data_T_G_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.897
```

```
_cell_length_b                  7.643
_cell_length_c                  10.792
_cell_angle_alpha                90.00
_cell_angle_beta                 108.39
_cell_angle_gamma                  90.00
_cell_volume                    696.376
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.03875 0.55467 -0.19050
N'2 N -0.17195 0.62435 -0.19554
H*3 H -0.16247 0.69669 -0.11396
N4 N -0.03013 0.43508 -0.28557
H*5 H 0.06668 0.44720 -0.31528
H*6 H -0.13273 0.42872 -0.36074
N7 N 0.10887 0.58516 -0.09733
H*8 H 0.10414 0.65252 -0.01796
H*9 H 0.18137 0.47961 -0.07408
C1+ C -0.10487 0.01414 0.72229
N'2+ N -0.24518 0.00208 0.63426
N'3+ N -0.22129 -0.09357 0.53615
N'4+ N -0.07277 -0.13805 0.56306
N5+ N 0.00280 -0.07077 0.68084
N6+ N -0.06200 0.10296 0.84773
O7+ O -0.16622 0.17676 0.87815
O8+ O 0.07949 0.09412 0.91219
H*9+ H 0.12072 -0.08551 0.72603

#END

data_T_G_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  11.454
_cell_length_b                  7.299
_cell_length_c                  9.722
_cell_angle_alpha                90.00
_cell_angle_beta                 63.18
_cell_angle_gamma                  90.00
_cell_volume                    725.353
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.49586 -0.39009 -0.65797
N'2 N 0.39365 -0.32001 -0.54757
H*3 H 0.31076 -0.35515 -0.55571
N4 N 0.62031 -0.34220 -0.67774
H*5 H 0.68519 -0.44703 -0.70747
H*6 H 0.61687 -0.26723 -0.58828
N7 N 0.49993 -0.51735 -0.76765
H*8 H 0.41331 -0.53679 -0.76978
H*9 H 0.57562 -0.50201 -0.87428
C1+ C 0.57363 0.05642 0.22024
N'2+ N 0.65020 -0.00684 0.08222
N'3+ N 0.77348 0.02174 0.06401
N'4+ N 0.77228 0.09914 0.18567
N5+ N 0.64623 0.12212 0.28596
N6+ N 0.43147 0.06022 0.29874
O7+ O 0.37288 -0.00185 0.23155
O8+ O 0.38353 0.12785 0.42897
H*9+ H 0.61658 0.17982 0.39134

#END

data_T_G_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 13.056
_cell_length_b                 11.018
_cell_length_c                 5.087
_cell_angle_alpha               90.00
_cell_angle_beta                106.90
_cell_angle_gamma                90.00
_cell_volume                   700.168
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.62405 -0.20460 0.10696
N'2 N 0.66875 -0.12297 -0.00276
```

H*3 H 0.66445 -0.03952 0.08039
N4 N 0.61073 -0.32222 0.00138
H*5 H 0.62433 -0.38904 0.14438
H*6 H 0.64991 -0.33527 -0.14148
N7 N 0.58506 -0.19129 0.33408
H*8 H 0.58033 -0.10431 0.39317
H*9 H 0.51839 -0.24009 0.32598
C1+ C 0.13382 0.21858 0.40364
N'2+ N 0.08885 0.16750 0.57519
N'3+ N 0.11122 0.04747 0.56687
N'4+ N 0.16744 0.02615 0.39752
N5+ N 0.18251 0.13375 0.29213
N6+ N 0.13473 0.34635 0.33303
O7+ O 0.08886 0.41743 0.44276
O8+ O 0.18325 0.37022 0.16451
H*9+ H 0.22405 0.14392 0.15326

#END

S38. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 5-nitrotetrazole (cocrystal form).

data_T_AG_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 14.056
_cell_length_b 9.619
_cell_length_c 6.698
_cell_angle_alpha 90.00
_cell_angle_beta 52.94
_cell_angle_gamma 90.00
_cell_volume 722.674
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.04703 0.19397 0.06920
N2 N 0.01158 0.18789 -0.08538
H*3 H -0.05193 0.25854 -0.04162
N'4 N 0.05904 0.07969 0.15382
N5 N 0.06603 0.32675 0.11834
H*6 H 0.09726 0.39518 -0.02359
H*7 H 0.11376 0.32413 0.18715

N8 N 0.10879 0.10494 0.28724
H*9 H 0.03892 0.10707 0.47368
H*10 H 0.15458 0.01680 0.26415
H*11 H -0.01201 0.08998 -0.09566
C1+ C 0.31832 0.05903 0.63235
N'2+ N 0.28415 0.09795 0.49013
N'3+ N 0.25755 -0.01755 0.43124
N4+ N 0.27671 -0.11906 0.53932
N'5+ N 0.31482 -0.07715 0.66760
N6+ N 0.35600 0.15751 0.73893
O7+ O 0.35548 0.28040 0.69329
O8+ O 0.38465 0.10822 0.86409
H*9+ H 0.26293 -0.22079 0.52369

#END

data_T_AG_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 9.920
_cell_length_b 7.677
_cell_length_c 11.187
_cell_angle_alpha 90.00
_cell_angle_beta 65.51
_cell_angle_gamma 90.00
_cell_volume 775.308
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.30032 0.60037 -0.32624
N2 N 0.25132 0.68993 -0.40924
H*3 H 0.19836 0.61344 -0.45013
N'4 N 0.43225 0.62974 -0.33437
N5 N 0.19893 0.48462 -0.24087
H*6 H 0.09176 0.52145 -0.21065
H*7 H 0.22766 0.45045 -0.16664
N8 N 0.45787 0.54029 -0.23161
H*9 H 0.51409 0.42826 -0.27200
H*10 H 0.53230 0.61559 -0.21418
H*11 H 0.33418 0.75989 -0.47773
C1+ C 0.19547 0.42673 0.19068

```
N'2+ N 0.11299 0.41538 0.12035
N'3+ N 0.19920 0.34227 0.00936
N4+ N 0.32765 0.31352 0.01807
N'5+ N 0.33161 0.36378 0.12941
N6+ N 0.14054 0.50157 0.32278
O7+ O 0.01313 0.55531 0.36887
O8+ O 0.22688 0.50374 0.37531
H*9+ H 0.41552 0.25717 -0.05559

#END

data_T_AG_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 18.592
_cell_length_b                 7.660
_cell_length_c                 10.846
_cell_angle_alpha               90.00
_cell_angle_beta                99.22
_cell_angle_gamma                90.00
_cell_volume                   1524.67
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.33593 0.35934 -0.42491
N2 N -0.35449 0.46319 -0.53087
H*3 H -0.38196 0.39823 -0.60540
N'4 N -0.27109 0.37087 -0.36102
N5 N -0.39085 0.25028 -0.39845
H*6 H -0.44179 0.29917 -0.42272
H*7 H -0.37983 0.20527 -0.30912
N8 N -0.26421 0.26856 -0.24735
H*9 H -0.24037 0.15284 -0.26502
H*10 H -0.22595 0.33151 -0.18540
H*11 H -0.31054 0.52766 -0.55261
C1+ C 0.59058 0.18869 0.02963
N'2+ N 0.54867 0.16790 -0.08342
```

```
N'3+ N 0.58858 0.07850 -0.14969
N4+ N 0.65173 0.05013 -0.07443
N'5+ N 0.65602 0.11616 0.03893
N6+ N 0.56644 0.28263 0.13322
O7+ O 0.50495 0.34373 0.11328
O8+ O 0.60987 0.29168 0.23048
H*9+ H 0.69325 -0.01723 -0.10254

#END

data_T_AG_4
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.216
_cell_length_b                 17.163
_cell_length_c                 10.928
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1540.97
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.52295 0.11405 0.38001
N2 N 0.42039 0.17826 0.36672
H*3 H 0.32888 0.18017 0.42899
N'4 N 0.56669 0.07536 0.28390
N5 N 0.56849 0.09769 0.49926
H*6 H 0.57915 0.14521 0.55370
H*7 H 0.66656 0.06148 0.50136
N8 N 0.68667 0.01640 0.31344
H*9 H 0.62554 -0.03523 0.32189
H*10 H 0.75498 0.01028 0.23629
H*11 H 0.37854 0.18308 0.27971
C1+ C 0.08912 0.15821 0.61656
N'2+ N -0.03877 0.11392 0.65175
N'3+ N -0.08896 0.07919 0.55225
```

N4+ N 0.00974 0.10389 0.46317
N'5+ N 0.12347 0.15343 0.49818
N6+ N 0.18227 0.20729 0.70082
O7+ O 0.13892 0.20683 0.80779
O8+ O 0.29513 0.24439 0.65681
H*9+ H -0.00209 0.08582 0.37516

#END

data_T_AG_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 15.523
_cell_length_b 8.271
_cell_length_c 5.989
_cell_angle_alpha 90.00
_cell_angle_beta 86.11
_cell_angle_gamma 90.00
_cell_volume 767.161
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.10549 0.22430 0.53182
N2 N 0.13303 0.29894 0.33065
H*3 H 0.18008 0.38256 0.34608
N'4 N 0.02369 0.20458 0.58045
N5 N 0.17107 0.17783 0.66370
H*6 H 0.22640 0.14414 0.57657
H*7 H 0.14927 0.09701 0.78263
N8 N 0.00766 0.10965 0.78238
H*9 H -0.00581 0.18946 0.91046
H*10 H -0.04915 0.05140 0.76304
H*11 H 0.08259 0.34412 0.25125
C1+ C 0.69263 -0.04299 -0.17091
N'2+ N 0.63052 -0.07138 -0.00611
N'3+ N 0.56989 -0.14975 -0.10183
N4+ N 0.59801 -0.16458 -0.31667
N'5+ N 0.67446 -0.09999 -0.36938
N6+ N 0.77302 0.04288 -0.13540
O7+ O 0.78238 0.08964 0.05501
O8+ O 0.82369 0.06025 -0.29917

H*9+ H 0.56307 -0.22135 -0.43062

#END

S39. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 5-nitrotetrazole (cocrystal form).

```
data_T_DAG_1
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 8.328
_cell_length_b                 8.421
_cell_length_c                 7.341
_cell_angle_alpha               98.58
_cell_angle_beta               119.44
_cell_angle_gamma              102.34
_cell_volume                   417.974
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.24877 0.14875 0.38176
N'2 N -0.30796 0.06758 0.48547
N3 N -0.25375 0.05866 0.20190
H*4 H -0.13408 0.11121 0.19860
N5 N -0.17354 0.32450 0.43466
N6 N -0.30100 -0.12075 0.15361
N7 N -0.30494 0.18188 0.65526
H*8 H -0.16795 0.21949 0.79421
H*9 H -0.25660 -0.15126 0.29690
H*10 H -0.44964 -0.17199 0.06273
H*11 H -0.39442 0.10837 0.68946
H*12 H -0.20087 0.36756 0.30396
H*13 H -0.21274 0.38390 0.52993
C1+ C 0.27563 0.37970 0.16295
N'2+ N 0.08134 0.29794 0.05995
N'3+ N 0.06560 0.18246 0.15648
N4+ N 0.24860 0.19997 0.31082
N'5+ N 0.38598 0.32148 0.32228
N6+ N 0.35846 0.52014 0.10515
O7+ O 0.24185 0.56238 -0.04464
O8+ O 0.53683 0.58275 0.21171
H*9+ H 0.27936 0.12523 0.41160

#END
```

```
data_T_DAG_2
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 8.830
_cell_length_b                 7.741
_cell_length_c                 7.148
_cell_angle_alpha               67.20
_cell_angle_beta                98.70
_cell_angle_gamma               99.70
_cell_volume                   441.98
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.17872 0.19963 -0.01056
N'2 N 0.04565 0.26167 -0.05732
N3 N 0.22315 0.08783 0.19091
H*4 H 0.33561 0.11990 0.23452
N5 N 0.28914 0.23672 -0.14465
N6 N 0.12879 0.06424 0.34506
N7 N 0.01631 0.36238 -0.27383
H*8 H 0.06253 0.50007 -0.30597
H*9 H 0.07414 0.18233 0.30146
H*10 H 0.04356 -0.04265 0.34633
H*11 H -0.09992 0.36509 -0.29961
H*12 H 0.35564 0.13141 -0.10846
H*13 H 0.24106 0.27958 -0.29158
C1+ C -0.34819 0.25808 0.32823
N'2+ N -0.44431 0.15290 0.23617
N'3+ N -0.36047 0.12449 0.11736
N4+ N -0.21984 0.21270 0.14321
N'5+ N -0.20550 0.29871 0.27346
N6+ N -0.39608 0.32220 0.47547
O7+ O -0.53064 0.27575 0.51363
O8+ O -0.29735 0.41649 0.54726
H*9+ H -0.13082 0.21334 0.06809

#END

data_T_DAG_3
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
```

```
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 7.576
_cell_length_b                 6.828
_cell_length_c                 8.258
_cell_angle_alpha               101.86
_cell_angle_beta                93.26
_cell_angle_gamma                94.15
_cell_volume                   415.835
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.77878 -0.24022 0.54869
N'2 N 0.72719 -0.41913 0.46592
N3 N 0.91942 -0.21089 0.67067
H*4 H 0.89864 -0.10719 0.77323
N5 N 0.70383 -0.06556 0.53098
N6 N 0.98841 -0.38150 0.71560
N7 N 0.58977 -0.41726 0.33805
H*8 H 0.47043 -0.42059 0.39005
H*9 H 0.88846 -0.49467 0.69766
H*10 H 1.07797 -0.43008 0.63210
H*11 H 0.58891 -0.55211 0.25784
H*12 H 0.79089 0.05859 0.55486
H*13 H 0.63242 -0.08549 0.41979
C1+ C 0.73543 0.14768 0.02267
N'2+ N 0.63594 0.17420 0.15514
N'3+ N 0.62865 0.00312 0.20305
N4+ N 0.72279 -0.11653 0.09860
N'5+ N 0.79268 -0.03392 -0.01682
N6+ N 0.77709 0.30437 -0.06986
O7+ O 0.71672 0.46559 -0.02154
O8+ O 0.86852 0.26021 -0.18722
H*9+ H 0.73917 -0.26026 0.10757

#END

data_T_DAG_4
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
```

```
_cell_length_a                 9.187
_cell_length_b                 12.064
_cell_length_c                 5.876
_cell_angle_alpha               134.06
_cell_angle_beta                83.99
_cell_angle_gamma                111.80
_cell_volume                   422.863
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25522 -0.52219 0.01643
N'2 N 0.31481 -0.38591 0.07909
N3 N 0.12587 -0.66616 -0.24991
H*4 H 0.04293 -0.72659 -0.20093
N5 N 0.30624 -0.54115 0.19747
N6 N 0.04938 -0.65282 -0.42274
N7 N 0.45428 -0.25584 0.34778
H*8 H 0.41482 -0.18837 0.55809
H*9 H 0.06010 -0.53086 -0.26470
H*10 H 0.11494 -0.66848 -0.58680
H*11 H 0.51283 -0.17380 0.32792
H*12 H 0.29262 -0.66081 0.06480
H*13 H 0.41945 -0.45150 0.33810
C1+ C 0.24285 -0.03451 0.00840
N'2+ N 0.13610 -0.03082 0.18814
N'3+ N 0.13257 -0.13926 0.19059
N4+ N 0.23593 -0.20217 0.01467
N'5+ N 0.30841 -0.14115 -0.10534
N6+ N 0.28339 0.06938 -0.05649
O7+ O 0.21501 0.16281 0.06156
O8+ O 0.38198 0.05356 -0.22290
H*9+ H 0.25696 -0.29035 -0.02355

#END

data_T_DAG_5
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 10.059
_cell_length_b                 10.961
_cell_length_c                 4.888
_cell_angle_alpha               62.72
_cell_angle_beta                106.00
```

```
_cell_angle_gamma              75.66
_cell_volume                  413.973
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.34816 -0.28147 0.70454
N'2 N 0.26237 -0.24389 0.40138
N3 N 0.46028 -0.22885 0.74916
H*4 H 0.55985 -0.30937 0.96688
N5 N 0.34281 -0.37550 1.00710
N6 N 0.49064 -0.15058 0.46673
N7 N 0.14674 -0.29976 0.40336
H*8 H 0.19433 -0.40842 0.46503
H*9 H 0.46797 -0.19049 0.31490
H*10 H 0.41142 -0.03936 0.31960
H*11 H 0.06572 -0.23607 0.15298
H*12 H 0.37161 -0.35032 1.18400
H*13 H 0.24078 -0.38240 0.95580
C1+ C 0.17824 0.23669 0.47347
N'2+ N 0.10169 0.21103 0.24606
N'3+ N 0.10332 0.07870 0.43437
N4+ N 0.17971 0.03169 0.76156
N'5+ N 0.22925 0.12604 0.80139
N6+ N 0.20328 0.37394 0.36992
O7+ O 0.15076 0.46780 0.06001
O8+ O 0.27445 0.38260 0.60234
H*9+ H 0.19814 -0.06916 0.96409

#END
```

S40. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 5-nitrotetrazole (cocrystal form).

```
data_T_TAG_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.267
_cell_length_b                 14.092
_cell_length_c                 8.981
_cell_angle_alpha               90.00
_cell_angle_beta                85.62
_cell_angle_gamma               90.00
```

```
_cell_volume                    917.027
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.61220 0.52227 0.18996
N'2 N 0.54917 0.45478 0.27790
N3 N 0.35459 0.46632 0.31958
N4 N 0.50008 0.59212 0.13446
N5 N 0.58937 0.67323 0.06965
N6 N 0.79817 0.52660 0.14541
N7 N 0.91057 0.44637 0.16442
H*8 H 0.32705 0.42139 0.40702
H*9 H 0.28224 0.44022 0.23503
H*10 H 0.38650 0.60305 0.20640
H*11 H 0.51222 0.69812 -0.01153
H*12 H 0.60257 0.72521 0.14713
H*13 H 0.83149 0.56385 0.05099
H*14 H 0.93756 0.44456 0.27413
H*15 H 0.83367 0.38675 0.14912
C1+ C 0.96569 0.19427 0.08936
N'2+ N 0.81921 0.24469 0.14800
N'3+ N 0.67942 0.21614 0.07636
N4+ N 0.74750 0.15082 -0.02063
N'5+ N 0.92592 0.13426 -0.01739
N6+ N 1.15220 0.20442 0.13845
O7+ O 1.17157 0.26205 0.23772
O8+ O 1.27206 0.15440 0.07587
H*9+ H 0.66766 0.11655 -0.09144

#END

data_T_TAG_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  8.782
_cell_length_b                  10.944
_cell_length_c                  19.119
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
_cell_volume                     1837.53
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.33444 0.31103 -0.34465
N'2 N 0.27307 0.40437 -0.37556
N3 N 0.23591 0.37765 -0.44753
N4 N 0.34994 0.19707 -0.37643
N5 N 0.44952 0.11239 -0.34397
N6 N 0.38636 0.32139 -0.27672
N7 N 0.33969 0.42187 -0.23558
H*8 H 0.21512 0.46026 -0.46989
H*9 H 0.13401 0.33213 -0.44862
H*10 H 0.35759 0.20666 -0.42939
H*11 H 0.40996 0.02681 -0.35357
H*12 H 0.55746 0.11993 -0.36317
H*13 H 0.39633 0.24202 -0.25006
H*14 H 0.40332 0.49505 -0.25090
H*15 H 0.23028 0.44390 -0.24918
C1+ C -0.15102 0.22883 0.59079
N'2+ N -0.22452 0.14839 0.63257
N'3+ N -0.12106 0.06943 0.65182
N4+ N 0.00796 0.10561 0.62113
N'5+ N -0.00409 0.20487 0.58231
N6+ N -0.22579 0.33338 0.55759
O7+ O -0.36167 0.34586 0.56936
O8+ O -0.14580 0.39894 0.52104
H*9+ H 0.10772 0.06000 0.62730

#END

data_T_TAG_3
_symmetry_cell_setting           monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   12.753
_cell_length_b                   10.293
_cell_length_c                   7.467
_cell_angle_alpha                90.00
```

```
_cell_angle_beta                71.50
_cell_angle_gamma               90.00
_cell_volume                    929.516
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.78889 0.48864 0.44064
N'2 N 0.89294 0.46754 0.35363
N3 N 0.93818 0.37303 0.45182
N4 N 0.72804 0.41963 0.60045
N5 N 0.62403 0.47171 0.70674
N6 N 0.73277 0.58206 0.37425
N7 N 0.77988 0.63113 0.18936
H*8 H 1.02158 0.38080 0.39337
H*9 H 0.91872 0.28212 0.41631
H*10 H 0.77854 0.38751 0.67318
H*11 H 0.57329 0.39681 0.76719
H*12 H 0.63122 0.53255 0.81001
H*13 H 0.64966 0.57198 0.41537
H*14 H 0.83894 0.69659 0.19404
H*15 H 0.82250 0.55748 0.10510
C1+ C 0.18847 0.71719 -0.06111
N'2+ N 0.11107 0.81080 -0.04043
N'3+ N 0.02136 0.76442 0.08182
N4+ N 0.04866 0.64676 0.12825
N'5+ N 0.15221 0.61214 0.04308
N6+ N 0.30239 0.72962 -0.18686
O7+ O 0.32593 0.83107 -0.27560
O8+ O 0.36390 0.63751 -0.19206
H*9+ H -0.00630 0.58847 0.22210

#END

data_T_TAG_4
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  11.871
_cell_length_b                  12.238
_cell_length_c                  6.724
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
```

```
_cell_angle_gamma                90.00
_cell_volume                     976.845
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.69911 0.15457 0.86991
N'2 N 0.67025 0.09091 1.01552
N3 N 0.73091 0.11696 1.19552
N4 N 0.77290 0.24230 0.89240
N5 N 0.81778 0.28875 0.71635
N6 N 0.65512 0.13783 0.68220
N7 N 0.55947 0.07034 0.65896
H*8 H 0.71803 0.05211 1.28725
H*9 H 0.69176 0.18170 1.26293
H*10 H 0.82735 0.22790 1.00684
H*11 H 0.83187 0.36943 0.74147
H*12 H 0.89175 0.25220 0.67726
H*13 H 0.65703 0.20321 0.59039
H*14 H 0.58679 -0.00854 0.66641
H*15 H 0.50898 0.08003 0.78120
C1+ C 0.16652 0.09402 0.67113
N'2+ N 0.11253 0.19096 0.65505
N'3+ N 0.00848 0.16643 0.61004
N4+ N 0.00486 0.05742 0.60129
N'5+ N 0.10135 0.00783 0.63823
N6+ N 0.28621 0.08410 0.72037
O7+ O 0.33741 0.16945 0.74739
O8+ O 0.32437 -0.00860 0.73013
H*9+ H -0.06689 0.01599 0.56863

#END

data_T_TAG_5
_symmetry_cell_setting           monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   7.258
_cell_length_b                   12.549
_cell_length_c                   10.279
_cell_angle_alpha                90.00
_cell_angle_beta                 74.94
_cell_angle_gamma                90.00
```

_cell_volume 904.063
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.12354 0.26858 0.13203
N'2 N 0.09901 0.18322 0.20572
N3 N 0.08636 0.08921 0.12749
N4 N 0.14960 0.26667 -0.00718
N5 N 0.12977 0.36471 -0.07064
N6 N 0.12722 0.36730 0.19073
N7 N 0.15161 0.37376 0.32246
H*8 H 0.03405 0.03137 0.19645
H*9 H 0.22192 0.06543 0.07928
H*10 H 0.08466 0.20138 -0.03447
H*11 H 0.21702 0.36317 -0.16551
H*12 H -0.00733 0.37620 -0.07563
H*13 H 0.19297 0.42578 0.12804
H*14 H 0.02302 0.35638 0.38727
H*15 H 0.23993 0.31307 0.33476
C1+ C 0.21531 0.12213 0.62870
N'2+ N 0.02827 0.09815 0.67702
N'3+ N -0.04684 0.11178 0.57564
N4+ N 0.09657 0.14288 0.47258
N'5+ N 0.26390 0.15073 0.50002
N6+ N 0.35319 0.11726 0.71022
O7+ O 0.29122 0.08980 0.82754
O8+ O 0.51805 0.14106 0.65381
H*9+ H 0.07789 0.15922 0.38012

#END

S41. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 5-(trinitromethyl)tetrazole (cocrystal form).
data_FTNM_NH3_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 6.125
_cell_length_b 11.781
_cell_length_c 12.639
_cell_angle_alpha 90.00
_cell_angle_beta 72.76

```
_cell_angle_gamma                90.00
_cell_volume                     871.038
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.12751 0.64491 -0.12221
H*2 H -0.01774 0.63468 -0.05786
H*3 H 0.20450 0.56744 -0.13746
H*4 H 0.07773 0.66544 -0.18992
C1+ C 0.61997 0.09429 0.31931
N2+ N 0.50866 0.17357 0.46889
N'3+ N 0.32449 0.12170 0.45638
N'4+ N 0.39331 0.07034 0.36092
N'5+ N 0.69780 0.15928 0.38612
C6+ C 0.75979 0.04936 0.21023
N7+ N 1.01945 0.05946 0.19411
O8+ O 1.12959 -0.02749 0.18397
O9+ O 1.08600 0.15680 0.19244
N10+ N 0.69908 -0.07785 0.20053
O11+ O 0.70005 -0.13492 0.28032
O12+ O 0.65844 -0.10726 0.11638
N13+ N 0.71756 0.11283 0.10955
O14+ O 0.53654 0.16252 0.12810
O15+ O 0.86852 0.10417 0.02255
H*16+ H 0.50379 0.22018 0.53707

#END

data_FTNM_NH3_2
_symmetry_cell_setting           monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   5.808
_cell_length_b                   8.059
_cell_length_c                   18.112
_cell_angle_alpha                90.00
_cell_angle_beta                 102.27
_cell_angle_gamma                90.00
_cell_volume                     828.397
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.76698 0.19512 0.41479
H*2 H 0.67320 0.12638 0.37142
H*3 H 0.67309 0.30085 0.41774
H*4 H 0.76864 0.13033 0.46321
C1+ C 0.29048 -0.10250 -0.14275
N2+ N 0.16330 0.13281 -0.14179
N'3+ N -0.00407 0.04952 -0.18914
N'4+ N 0.07481 -0.10163 -0.19023
N'5+ N 0.35078 0.04428 -0.11110
C6+ C 0.43636 -0.25568 -0.12891
N7+ N 0.63895 -0.24098 -0.05835
O8+ O 0.63718 -0.33442 -0.00602
O9+ O 0.78279 -0.13475 -0.06387
N10+ N 0.27671 -0.40514 -0.11808
O11+ O 0.15177 -0.37933 -0.07345
O12+ O 0.29231 -0.53003 -0.15403
N13+ N 0.55734 -0.30063 -0.19552
O14+ O 0.46611 -0.24323 -0.25669
O15+ O 0.72781 -0.39092 -0.17949
H*16+ H 0.14728 0.25488 -0.13008

#END

data_FTNM_NH3_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 15.229
_cell_length_b                 9.365
_cell_length_c                 6.046
_cell_angle_alpha               90.00
_cell_angle_beta                95.02
_cell_angle_gamma                 90.00
_cell_volume                   858.97
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.46178 0.11342 -0.26577
H*2 H 0.47168 0.19240 -0.37685
```

H*3 H 0.42619 0.03562 -0.35048
H*4 H 0.52204 0.07092 -0.21758
C1+ C 0.25688 0.60666 -0.28052
N2+ N 0.14811 0.66742 -0.13099
N'3+ N 0.13088 0.53475 -0.20184
N'4+ N 0.20010 0.49429 -0.29773
N'5+ N 0.22577 0.71768 -0.17508
C6+ C 0.34454 0.60025 -0.37117
N7+ N 0.40698 0.72073 -0.27936
O8+ O 0.47403 0.68666 -0.16917
O9+ O 0.38116 0.83981 -0.33159
N10+ N 0.38833 0.45335 -0.31142
O11+ O 0.38767 0.42065 -0.11738
O12+ O 0.41844 0.38743 -0.46000
N13+ N 0.33935 0.61545 -0.62929
O14+ O 0.26891 0.58573 -0.72804
O15+ O 0.40686 0.65296 -0.70491
H*16+ H 0.10489 0.72513 -0.04879

#END

data_FTNM_NH3_4
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P 21 21 21'
_symmetry_Int_Tables_number 19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 6.350
_cell_length_b 10.989
_cell_length_c 11.879
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 828.918
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.79326 -0.08452 0.29108
H*2 H 0.86129 -0.12761 0.22439
H*3 H 0.63440 -0.09110 0.28048
H*4 H 0.83012 -0.13369 0.36109
C1+ C -0.22912 0.61349 -0.08536
N2+ N -0.26679 0.78159 -0.15463
N'3+ N -0.06475 0.77668 -0.12455

N'4+ N -0.03816 0.66933 -0.08018
N'5+ N -0.37679 0.68238 -0.13242
C6+ C -0.26103 0.48756 -0.04260
N7+ N -0.46895 0.43049 -0.08523
O8+ O -0.45727 0.34099 -0.14454
O9+ O -0.62570 0.48310 -0.05248
N10+ N -0.07350 0.40618 -0.08101
O11+ O -0.03247 0.41424 -0.18050
O12+ O 0.01115 0.34378 -0.01002
N13+ N -0.27180 0.48005 0.08859
O14+ O -0.19030 0.56359 0.13923
O15+ O -0.35730 0.39020 0.12644
H*16+ H -0.33084 0.85588 -0.19209

#END

data_FTNM_NH3_5
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P 21 21 21'
_symmetry_Int_Tables_number 19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 12.183
_cell_length_b 5.836
_cell_length_c 12.220
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 868.842
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.78864 -0.14481 -0.10317
H*2 H 0.72297 -0.23467 -0.07444
H*3 H 0.82067 -0.23689 -0.16642
H*4 H 0.75877 0.00354 -0.13553
C1+ C 0.19849 0.05865 0.87430
N2+ N 0.05329 -0.08353 0.92123
N'3+ N 0.03874 -0.02526 0.81677
N'4+ N 0.13123 0.06576 0.78551
N'5+ N 0.15135 -0.03566 0.96137
C6+ C 0.31290 0.14744 0.87000
N7+ N 0.38310 0.06435 0.96773
O8+ O 0.46193 -0.05559 0.94819

O9+ O 0.35064 0.13279 1.05588
N10+ N 0.36810 0.06733 0.76159
O11+ O 0.35791 -0.13582 0.74310
O12+ O 0.41512 0.21120 0.70749
N13+ N 0.31956 0.41467 0.87273
O14+ O 0.23748 0.51566 0.84378
O15+ O 0.40693 0.49390 0.90165
H*16+ H -0.00645 -0.15958 0.96628

#END

S42. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 5-(trinitromethyl)tetrazole (cocrystal form).

data_FTNM_NH2OH_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 19.435
_cell_length_b 7.886
_cell_length_c 5.889
_cell_angle_alpha 90.00
_cell_angle_beta 104.49
_cell_angle_gamma 90.00
_cell_volume 873.864
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.51324 -0.17709 0.64041
H*2 H 0.52557 -0.05583 0.69756
H*3 H 0.55924 -0.24482 0.69551
O4 O 0.50318 -0.16590 0.38919
H*5 H 0.45607 -0.21191 0.33018
C1+ C 0.13132 0.14252 0.23171
N2+ N 0.07907 -0.08244 0.21949
N'3+ N 0.08860 -0.06202 0.00476
N'4+ N 0.12215 0.08155 0.01003
N'5+ N 0.10472 0.04098 0.36842
C6+ C 0.16835 0.30604 0.30585
N7+ N 0.19047 0.32652 0.57561
O8+ O 0.25336 0.33631 0.67007
O9+ O 0.14051 0.33212 0.66490
N10+ N 0.23601 0.31654 0.21000

```
O11+ O 0.27327 0.19109 0.24845
O12+ O 0.24502 0.44568 0.10946
N13+ N 0.12181 0.46472 0.21182
O14+ O 0.07334 0.44167 0.03939
O15+ O 0.13972 0.59561 0.31848
H*16+ H 0.05418 -0.18537 0.26502

#END

data_FTNM_NH2OH_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 21.282
_cell_length_b                 7.659
_cell_length_c                 11.206
_cell_angle_alpha               90.00
_cell_angle_beta                73.63
_cell_angle_gamma                 90.00
_cell_volume                   1752.52
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.48686 -0.18707 0.44500
H*2 H 0.47641 -0.06285 0.42322
H*3 H 0.44364 -0.25400 0.46307
O4 O 0.49820 -0.16922 0.56569
H*5 H 0.54125 -0.21926 0.55233
C1+ C 0.12414 0.16093 0.25125
N2+ N 0.07330 -0.06764 0.28439
N'3+ N 0.08254 -0.03642 0.16366
N'4+ N 0.11517 0.10958 0.14100
N'5+ N 0.09828 0.05085 0.34365
C6+ C 0.16015 0.32389 0.26229
N7+ N 0.18053 0.33083 0.38424
O8+ O 0.23854 0.33399 0.37607
O9+ O 0.13447 0.33394 0.47750
N10+ N 0.22274 0.33701 0.14984
```

O11+ O 0.25556 0.20496 0.13071
O12+ O 0.23269 0.47428 0.09375
N13+ N 0.11923 0.49315 0.26212
O14+ O 0.07444 0.47970 0.21551
O15+ O 0.13721 0.62167 0.30663
H*16+ H 0.04909 -0.17472 0.32731

#END

data_FTNM_NH2OH_3
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 7.726
_cell_length_b 10.080
_cell_length_c 5.854
_cell_angle_alpha 75.78
_cell_angle_beta 92.87
_cell_angle_gamma 96.69
_cell_volume 438.811
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.31916 0.47596 0.64022
H*2 H -0.26003 0.38754 0.69402
H*3 H -0.44454 0.45059 0.69640
O4 O -0.33587 0.49615 0.38728
H*5 H -0.27854 0.58796 0.33038
C1+ C 0.10722 0.24073 0.25199
N2+ N -0.10185 0.35011 0.22197
N'3+ N -0.08759 0.32700 0.00945
N'4+ N 0.04574 0.25675 0.02610
N'5+ N 0.01591 0.29852 0.38029
C6+ C 0.26044 0.16425 0.33892
N7+ N 0.27654 0.12525 0.61110
O8+ O 0.26404 0.00400 0.71019
O9+ O 0.30228 0.22402 0.69734
N10+ N 0.24431 0.03030 0.24832
O11+ O 0.10328 -0.03733 0.28115
O12+ O 0.37080 0.00648 0.15676
N13+ N 0.43800 0.24783 0.25210
O14+ O 0.43053 0.34001 0.07524
O15+ O 0.56569 0.21030 0.36817
H*16+ H -0.19645 0.40299 0.25922

```
#END
data_FTNM_NH2OH_4
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 7.814
_cell_length_b                 6.755
_cell_length_c                 12.508
_cell_angle_alpha               44.41
_cell_angle_beta                96.13
_cell_angle_gamma              105.71
_cell_volume                   441.06
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.33739 -0.29912 0.09916
H*2 H 0.28209 -0.43428 0.20982
H*3 H 0.47292 -0.26164 0.10135
O4 O 0.30741 -0.01990 0.01730
H*5 H 0.24483 0.02319 -0.06533
C1+ C 0.06682 -0.03873 0.73253
N2+ N -0.09900 0.02012 0.81761
N'3+ N -0.20097 -0.03169 0.74331
N'4+ N -0.09654 -0.07037 0.68837
N'5+ N 0.06904 0.01791 0.81493
C6+ C 0.22260 -0.06939 0.69127
N7+ N 0.37679 -0.10863 0.78817
O8+ O 0.41729 -0.33763 0.87200
O9+ O 0.44301 0.10289 0.76748
N10+ N 0.16034 -0.34102 0.71647
O11+ O 0.07344 -0.56358 0.84082
O12+ O 0.20380 -0.30604 0.61263
N13+ N 0.30803 0.20401 0.51958
O14+ O 0.21142 0.35769 0.43169
O15+ O 0.46137 0.23163 0.49119
H*16+ H -0.14721 0.05747 0.87244

#END

data_FTNM_NH2OH_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
```

```
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.838
_cell_length_b                 16.477
_cell_length_c                 6.261
_cell_angle_alpha               90.00
_cell_angle_beta                85.83
_cell_angle_gamma                 90.00
_cell_volume                   909.336
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.40792 0.18286 0.28673
H*2 H 0.40233 0.23223 0.38585
H*3 H 0.51733 0.18088 0.22163
O4 O 0.32156 0.20708 0.10993
H*5 H 0.24706 0.16439 0.10576
C1+ C 0.10065 0.62069 -0.22988
N2+ N -0.10482 0.67710 -0.21710
N'3+ N -0.08820 0.64456 -0.41230
N'4+ N 0.04293 0.60806 -0.42271
N'5+ N 0.00925 0.66405 -0.09624
C6+ C 0.25067 0.58739 -0.18046
N7+ N 0.27381 0.58892 0.06205
O8+ O 0.28877 0.52452 0.15172
O9+ O 0.27571 0.65687 0.13716
N10+ N 0.26453 0.49820 -0.26190
O11+ O 0.15590 0.45600 -0.20785
O12+ O 0.37956 0.47968 -0.36808
N13+ N 0.38762 0.63549 -0.28967
O14+ O 0.36110 0.67478 -0.44658
O15+ O 0.50726 0.62742 -0.20856
H*16+ H -0.19835 0.70923 -0.16529

#END
```

S43. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 5-(trinitromethyl)tetrazole (cocrystal form).

```
data_FTNM_N2H4_1
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
```

```
_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
_cell_length_a                 8.010
_cell_length_b                 6.192
_cell_length_c                 17.845
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   885.075
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.53894 0.52946 0.72781
H*2 H 0.60418 0.66707 0.73923
H*3 H 0.62291 0.40958 0.71803
N4 N 0.43744 0.55119 0.66186
H*5 H 0.32439 0.60918 0.67820
H*6 H 0.48709 0.65815 0.62453
C1+ C 0.45757 -0.03194 0.09831
N2+ N 0.22343 -0.15804 0.09031
N'3+ N 0.31800 -0.28422 0.04718
N'4+ N 0.46854 -0.20557 0.05186
N'5+ N 0.30380 0.00162 0.12367
C6+ C 0.60643 0.10059 0.11767
N7+ N 0.57580 0.24763 0.18639
O8+ O 0.65982 0.21691 0.24187
O9+ O 0.46830 0.38302 0.17633
N10+ N 0.75649 -0.05167 0.13472
O11+ O 0.72419 -0.19643 0.17821
O12+ O 0.88803 -0.01205 0.10403
N13+ N 0.66199 0.25539 0.05320
O14+ O 0.61705 0.20520 -0.00937
O15+ O 0.74707 0.40798 0.07217
H*16+ H 0.09917 -0.18337 0.09711

#END

data_FTNM_N2H4_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21'
_symmetry_Int_Tables_number      4
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,-z
```

```
_cell_length_a                 7.874
_cell_length_b                 6.286
_cell_length_c                 10.048
_cell_angle_alpha               90.00
_cell_angle_beta               115.91
_cell_angle_gamma                90.00
_cell_volume                   447.344
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.43864 0.17932 -0.05453
H*2 H 0.39417 0.04751 -0.01951
H*3 H 0.33488 0.29064 -0.08380
N4 N 0.47023 0.13631 -0.18236
H*5 H 0.60661 0.08857 -0.14595
H*6 H 0.38581 0.01683 -0.24561
C1+ C -0.20519 0.66712 0.69527
N2+ N -0.45082 0.52805 0.67056
N'3+ N -0.39269 0.41243 0.58710
N'4+ N -0.23516 0.49948 0.60204
N'5+ N -0.33933 0.68866 0.74076
C6+ C -0.03630 0.80628 0.73973
N7+ N -0.00298 0.94532 0.87597
O8+ O 0.14149 0.91778 0.98778
O9+ O -0.12903 1.07190 0.85420
N10+ N 0.14144 0.66556 0.77647
O11+ O 0.15751 0.51881 0.85961
O12+ O 0.24464 0.71480 0.72059
N13+ N -0.05007 0.96553 0.61605
O14+ O -0.15857 0.91644 0.49061
O15+ O 0.05183 1.12024 0.65793
H*16+ H -0.57134 0.49458 0.67973

#END

data_FTNM_N2H4_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 10.954
_cell_length_b                 14.167
_cell_length_c                 6.067
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 102.62
_cell_angle_gamma                90.00
_cell_volume                     918.763
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.01104 0.09924 0.16246
H*2 H 0.05509 0.05152 0.14076
H*3 H -0.09305 0.06391 0.15021
N4 N -0.03110 0.17091 -0.00922
H*5 H 0.02975 0.22441 0.04611
H*6 H -0.01361 0.14679 -0.15773
C1+ C 0.71615 0.03332 0.41264
N2+ N 0.74506 0.17294 0.48554
N'3+ N 0.73515 0.16675 0.26312
N'4+ N 0.71637 0.07766 0.21384
N'5+ N 0.73377 0.09201 0.58754
C6+ C 0.69652 -0.07034 0.42413
N7+ N 0.66449 -0.10100 0.64960
O8+ O 0.56295 -0.13645 0.64219
O9+ O 0.74807 -0.08628 0.81389
N10+ N 0.58785 -0.10068 0.22558
O11+ O 0.49431 -0.05272 0.20599
O12+ O 0.60617 -0.16771 0.11277
N13+ N 0.81401 -0.12947 0.40418
O14+ O 0.88857 -0.09015 0.31391
O15+ O 0.81750 -0.20934 0.47738
H*16+ H 0.75977 0.23523 0.56978

#END

data_FTNM_N2H4_4
_symmetry_cell_setting           orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   7.697
_cell_length_b                   11.897
_cell_length_c                   9.632
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
```

```
_cell_volume                    882.014
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.46667 0.23239 -0.18813
H*2 H 0.52875 0.28217 -0.25867
H*3 H 0.34006 0.25664 -0.18481
N4 N 0.53699 0.24512 -0.05086
H*5 H 0.63503 0.18849 -0.04026
H*6 H 0.58778 0.32332 -0.03537
C1+ C -0.04627 0.56080 -0.04577
N2+ N -0.21995 0.51512 0.10342
N'3+ N -0.27282 0.46239 -0.01113
N'4+ N -0.16252 0.49072 -0.10762
N'5+ N -0.07921 0.57751 0.08804
C6+ C 0.10156 0.61066 -0.12400
N7+ N 0.24230 0.66017 -0.02702
O8+ O 0.38597 0.61851 -0.03036
O9+ O 0.19142 0.73851 0.04297
N10+ N 0.18590 0.51858 -0.21713
O11+ O 0.21763 0.43151 -0.15660
O12+ O 0.21182 0.54194 -0.33790
N13+ N 0.04628 0.70929 -0.22153
O14+ O -0.10542 0.71066 -0.25584
O15+ O 0.16158 0.77330 -0.25506
H*16+ H -0.28292 0.50753 0.19551

#END

data_FTNM_N2H4_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  8.426
_cell_length_b                  19.191
_cell_length_c                  5.890
_cell_angle_alpha                 90.00
_cell_angle_beta                 72.10
_cell_angle_gamma                   90.00
_cell_volume                    906.33
loop_
_atom_site_label
```

_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.73821 0.35443 1.02572
H*2 H 0.69072 0.40268 1.07982
H*3 H 0.83886 0.36059 0.87839
N4 N 0.62058 0.31087 0.96034
H*5 H 0.55231 0.28533 1.10968
H*6 H 0.54014 0.33918 0.89828
C1+ C 0.13606 0.13363 0.90846
N2+ N -0.06087 0.18668 0.86159
N'3+ N 0.06701 0.20133 0.66890
N'4+ N 0.19410 0.16758 0.69623
N'5+ N -0.02520 0.14463 1.01681
C6+ C 0.24635 0.08878 1.00113
N7+ N 0.14672 0.04053 1.20574
O8+ O 0.15949 -0.02185 1.17303
O9+ O 0.06535 0.07174 1.38275
N10+ N 0.35707 0.04309 0.79418
O11+ O 0.28015 0.01312 0.67988
O12+ O 0.50553 0.04157 0.76784
N13+ N 0.36644 0.13113 1.10510
O14+ O 0.39456 0.19061 1.03420
O15+ O 0.42175 0.09975 1.24294
H*16+ H -0.17690 0.20622 0.88650

#END

S44. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 5-(trinitromethyl)tetrazole (cocrystal form).
data_FTNM_G_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.800
_cell_length_b 18.463
_cell_length_c 7.108
_cell_angle_alpha 90.00
_cell_angle_beta 83.59
_cell_angle_gamma 90.00
_cell_volume 1017.23
loop_
_atom_site_label
_atom_site_type_symbol

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.44287 0.17982 0.18473
N'2 N 0.42664 0.11365 0.23973
H*3 H 0.30057 0.09774 0.25348
N4 N 0.60228 0.21448 0.17753
H*5 H 0.63156 0.24708 0.06373
H*6 H 0.69855 0.17962 0.19889
N7 N 0.31470 0.22474 0.12568
H*8 H 0.19351 0.20494 0.15256
H*9 H 0.32349 0.27765 0.16156
C1+ C -0.15772 0.57513 -0.21493
N2+ N -0.35875 0.50551 -0.22673
N'3+ N -0.43062 0.57103 -0.21037
N'4+ N -0.30327 0.61624 -0.20297
N'5+ N -0.18897 0.50478 -0.23063
C6+ C 0.01602 0.60814 -0.21204
N7+ N 0.16330 0.55506 -0.28061
O8+ O 0.25647 0.57067 -0.42285
O9+ O 0.16993 0.50225 -0.17967
N10+ N 0.03062 0.67641 -0.34156
O11+ O -0.01400 0.66639 -0.49764
O12+ O 0.08428 0.73159 -0.27645
N13+ N 0.05321 0.63301 -0.01048
O14+ O -0.07268 0.64414 0.10224
O15+ O 0.20433 0.63993 0.01163
H*16+ H -0.42928 0.45973 -0.23607

#END

data_FTNM_G_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 29.406
_cell_length_b                 9.430
_cell_length_c                 7.692
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
```

```
_cell_volume                    2132.98
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.57205 0.02486 0.73675
N'2 N 0.53711 -0.05422 0.76237
H*3 H 0.54580 -0.14613 0.82402
N4 N 0.56834 0.14793 0.63732
H*5 H 0.58607 0.23225 0.68304
H*6 H 0.53557 0.17152 0.60881
N7 N 0.61613 0.00391 0.80011
H*8 H 0.62155 -0.09291 0.85282
H*9 H 0.64144 0.03453 0.71883
C1+ C 0.12263 -0.03290 0.24739
N2+ N 0.05353 -0.02203 0.23586
N'3+ N 0.06384 -0.15102 0.17698
N'4+ N 0.10803 -0.15962 0.18390
N'5+ N 0.08882 0.05618 0.28192
C6+ C 0.17178 -0.00268 0.27476
N7+ N 0.17969 0.12843 0.39177
O8+ O 0.19883 0.11048 0.52961
O9+ O 0.16568 0.23844 0.32933
N10+ N 0.19481 -0.13398 0.36044
O11+ O 0.17466 -0.17973 0.48617
O12+ O 0.22982 -0.17672 0.29574
N13+ N 0.19800 0.02877 0.10238
O14+ O 0.18074 -0.01689 -0.02955
O15+ O 0.23341 0.09348 0.11850
H*16+ H 0.02100 0.01308 0.24504

#END

data_FTNM_G_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  11.270
_cell_length_b                  16.751
_cell_length_c                  5.968
_cell_angle_alpha                 90.00
_cell_angle_beta                 71.89
_cell_angle_gamma                   90.00
```

```
_cell_volume                    1070.85
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.11130 0.54273 0.68830
N'2 N 0.06645 0.47165 0.70843
H*3 H 0.07941 0.44273 0.84951
N4 N 0.11561 0.58910 0.49191
H*5 H 0.09409 0.64750 0.52658
H*6 H 0.06835 0.56355 0.39126
N7 N 0.15864 0.58302 0.84745
H*8 H 0.17235 0.54805 0.97537
H*9 H 0.23171 0.61981 0.77303
C1+ C 0.87299 0.14138 0.03875
N2+ N 0.71654 0.10221 0.29027
N'3+ N 0.71177 0.06891 0.09041
N'4+ N 0.81159 0.09337 -0.07236
N'5+ N 0.81507 0.14788 0.26875
C6+ C 0.99312 0.18063 -0.09119
N7+ N 1.06300 0.21287 0.07579
O8+ O 1.16415 0.18438 0.05995
O9+ O 1.00707 0.26537 0.20688
N10+ N 1.07855 0.11949 -0.26443
O11+ O 1.08782 0.05567 -0.17510
O12+ O 1.12683 0.14084 -0.46649
N13+ N 0.97684 0.25391 -0.24087
O14+ O 0.88137 0.25525 -0.29420
O15+ O 1.06251 0.30127 -0.29213
H*16+ H 0.64966 0.09290 0.44708

#END

data_FTNM_G_4
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                  7.890
_cell_length_b                  7.488
_cell_length_c                  8.924
_cell_angle_alpha                86.19
_cell_angle_beta                 95.45
_cell_angle_gamma                92.27
_cell_volume                    523.395
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.45661 0.24929 0.39590
N'2 N 0.41551 0.27338 0.25342
H*3 H 0.29205 0.23328 0.22564
N4 N 0.62496 0.27679 0.45488
H*5 H 0.63957 0.33741 0.55374
H*6 H 0.69866 0.33419 0.37673
N7 N 0.34857 0.19726 0.50768
H*8 H 0.23104 0.15338 0.46779
H*9 H 0.40099 0.11699 0.59435
C1+ C 0.79110 0.28425 -0.13359
N2+ N 0.60368 0.29849 0.00668
N'3+ N 0.52258 0.29671 -0.13123
N'4+ N 0.64109 0.28729 -0.22236
N'5+ N 0.77120 0.29069 0.01208
C6+ C 0.95715 0.27296 -0.19817
N7+ N 1.10294 0.22031 -0.07689
O8+ O 1.17158 0.08018 -0.08706
O9+ O 1.13407 0.32995 0.01723
N10+ N 0.93996 0.13153 -0.31953
O11+ O 0.87514 -0.01062 -0.27797
O12+ O 0.99204 0.17518 -0.44062
N13+ N 1.01840 0.45359 -0.27668
O14+ O 0.90807 0.55917 -0.31780
O15+ O 1.16978 0.46843 -0.29096
H*16+ H 0.54120 0.30478 0.10038

#END

data_FTNM_G_5
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 11.058
_cell_length_b                 7.213
_cell_length_c                 13.782
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1099.27
loop_
```

_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.48236 0.30495 0.67846
N'2 N 0.39256 0.41793 0.67747
H*3 H 0.35355 0.42410 0.61045
N4 N 0.55631 0.29185 0.76010
H*5 H 0.58264 0.16142 0.77752
H*6 H 0.52223 0.36289 0.81733
N7 N 0.51808 0.18412 0.60440
H*8 H 0.47701 0.20693 0.53991
H*9 H 0.60859 0.16537 0.59802
C1+ C -0.05020 -0.05475 0.61056
N2+ N -0.21261 -0.05145 0.68021
N'3+ N -0.23266 0.03418 0.59603
N'4+ N -0.12938 0.03283 0.55051
N'5+ N -0.10055 -0.11011 0.69314
C6+ C 0.07848 -0.08395 0.58292
N7+ N 0.14187 -0.22952 0.64777
O8+ O 0.17834 -0.37010 0.60948
O9+ O 0.14905 -0.18405 0.73247
N10+ N 0.08487 -0.14937 0.47534
O11+ O 0.01693 -0.27630 0.45619
O12+ O 0.15545 -0.07005 0.42232
N13+ N 0.15701 0.09537 0.59123
O14+ O 0.10211 0.24093 0.58834
O15+ O 0.26521 0.07070 0.59794
H*16+ H -0.27864 -0.07053 0.73036

#END

S45. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 5-(trinitromethyl)tetrazole (cocrystal form).
data_FTNM_AG_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 9.027
_cell_length_b 8.076
_cell_length_c 7.899
_cell_angle_alpha 82.08
_cell_angle_beta 109.22
_cell_angle_gamma 85.72
_cell_volume 534.119
loop_

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.27353 0.52080 0.09301
N2 N 0.22676 0.51673 -0.09303
H*3 H 0.31539 0.52687 -0.14475
N'4 N 0.18478 0.61192 0.15355
N5 N 0.41569 0.42361 0.19726
H*6 H 0.43837 0.31755 0.15006
H*7 H 0.42787 0.40412 0.33151
N8 N 0.24268 0.58628 0.35069
H*9 H 0.30608 0.68321 0.38783
H*10 H 0.14480 0.60723 0.38566
H*11 H 0.13046 0.60198 -0.16455
C1+ C 0.19780 0.13562 0.37855
N2+ N 0.08005 0.19517 0.10528
N'3+ N 0.20549 0.08700 0.12354
N'4+ N 0.28197 0.04747 0.29806
N'5+ N 0.06902 0.22991 0.25969
C6+ C 0.24866 0.12231 0.57980
N7+ N 0.11534 0.19312 0.64276
O8+ O 0.06727 0.09629 0.73801
O9+ O 0.07351 0.34320 0.58899
N10+ N 0.30215 -0.06616 0.67063
O11+ O 0.20892 -0.16077 0.60616
O12+ O 0.42814 -0.09977 0.79424
N13+ N 0.39074 0.22129 0.65945
O14+ O 0.47212 0.24984 0.56603
O15+ O 0.40686 0.25681 0.80827
H*16+ H -0.00101 0.24643 -0.01802

#END

data_FTNM_AG_2
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 10.845
_cell_length_b                 8.018
_cell_length_c                 6.951
_cell_angle_alpha               99.45
_cell_angle_beta                92.80
_cell_angle_gamma               95.85
_cell_volume                   591.792
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25503 0.17130 0.51060
N2 N 0.35651 0.10762 0.59259
H*3 H 0.37927 0.15969 0.73459
N'4 N 0.26037 0.21073 0.33783
N5 N 0.15561 0.18670 0.62741
H*6 H 0.14430 0.09747 0.71465
H*7 H 0.07706 0.20003 0.54771
N8 N 0.14240 0.25648 0.26808
H*9 H 0.14839 0.38644 0.29367
H*10 H 0.13940 0.22368 0.11993
H*11 H 0.43062 0.11429 0.50951
C1+ C 0.66696 0.26724 0.13577
N2+ N 0.47955 0.24888 0.15616
N'3+ N 0.49496 0.21238 -0.03462
N'4+ N 0.61467 0.22335 -0.04993
N'5+ N 0.58354 0.28382 0.26937
C6+ C 0.80408 0.29112 0.17775
N7+ N 0.84177 0.29224 0.39550
O8+ O 0.90075 0.18041 0.43503
O9+ O 0.80770 0.40999 0.50573
N10+ N 0.86254 0.14492 0.05035
O11+ O 0.81225 0.00377 0.05641
O12+ O 0.95066 0.18460 -0.03991
N13+ N 0.86703 0.46250 0.13063
O14+ O 0.80906 0.52702 0.01415
O15+ O 0.96860 0.51197 0.21276
H*16+ H 0.39429 0.24921 0.21013

#END

data_FTNM_AG_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 14.820
_cell_length_b                 12.089
_cell_length_c                 6.044
_cell_angle_alpha               90.00
_cell_angle_beta                85.37
_cell_angle_gamma                 90.00
```

```
_cell_volume                    1079.3
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.07226 0.73581 0.40054
N2 N 0.01441 0.73753 0.22963
H*3 H -0.00493 0.81468 0.18733
N'4 N 0.05831 0.66465 0.55944
N5 N 0.14099 0.81364 0.38182
H*6 H 0.16399 0.83171 0.22354
H*7 H 0.19056 0.79458 0.48257
N8 N 0.13035 0.66673 0.70787
H*9 H 0.10806 0.71416 0.84138
H*10 H 0.13324 0.58841 0.76885
H*11 H -0.03935 0.68648 0.26229
C1+ C 0.72611 0.00275 0.19193
N2+ N 0.60493 0.08128 0.24965
N'3+ N 0.62170 0.08213 0.02966
N'4+ N 0.69911 0.03189 -0.00986
N'5+ N 0.66761 0.03273 0.35931
C6+ C 0.81247 -0.05747 0.21430
N7+ N 0.81705 -0.10913 0.44726
O8+ O 0.82180 -0.20899 0.46003
O9+ O 0.81612 -0.04131 0.59578
N10+ N 0.82271 -0.15111 0.03705
O11+ O 0.75606 -0.20893 0.03024
O12+ O 0.89442 -0.15757 -0.07396
N13+ N 0.89798 0.01796 0.17827
O14+ O 0.88865 0.10188 0.07235
O15+ O 0.96549 -0.01618 0.25655
H*16+ H 0.54811 0.11510 0.32672

#END

data_FTNM_AG_4
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
```

```
_cell_length_a                 18.218
_cell_length_b                 7.239
_cell_length_c                 16.291
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   2148.46
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.72872 0.79238 0.57941
N2 N 0.69675 0.85215 0.65253
H*3 H 0.72189 0.80299 0.70363
N'4 N 0.68700 0.73628 0.52019
N5 N 0.80466 0.79907 0.57792
H*6 H 0.82671 0.90353 0.61117
H*7 H 0.82394 0.79044 0.51940
N8 N 0.72895 0.69922 0.44644
H*9 H 0.73805 0.55985 0.44470
H*10 H 0.69378 0.72418 0.39915
H*11 H 0.64191 0.82785 0.65321
C1+ C 0.04770 0.25169 0.62577
N2+ N -0.03728 0.22574 0.54539
N'3+ N 0.02295 0.21889 0.49905
N'4+ N 0.07789 0.23503 0.54976
N'5+ N -0.02518 0.24575 0.62487
C6+ C 0.09389 0.27229 0.70054
N7+ N 0.05030 0.23612 0.78043
O8+ O 0.06892 0.10682 0.82288
O9+ O 0.00108 0.34620 0.79227
N10+ N 0.15931 0.13416 0.69604
O11+ O 0.14152 -0.02288 0.67924
O12+ O 0.22019 0.19457 0.70964
N13+ N 0.12720 0.46990 0.71041
O14+ O 0.13188 0.56049 0.64796
O15+ O 0.14622 0.51127 0.77936
H*16+ H -0.08851 0.21572 0.52135

#END

data_FTNM_AG_5
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.271
_cell_length_b 10.072
_cell_length_c 10.717
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1108.67
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.02690 0.31685 0.13688
N2 N -0.01724 0.25418 0.24495
H*3 H -0.05241 0.16136 0.23020
N'4 N -0.00406 0.43954 0.11704
N5 N 0.10174 0.23805 0.05902
H*6 H 0.15662 0.16949 0.10398
H*7 H 0.15205 0.29430 -0.00343
N8 N 0.06179 0.49210 0.00813
H*9 H -0.00272 0.48687 -0.06440
H*10 H 0.07240 0.59097 0.02520
H*11 H -0.08137 0.31191 0.29227
C1+ C 0.44400 0.06101 0.34144
N2+ N 0.24786 0.04021 0.32167
N'3+ N 0.28865 0.08924 0.21298
N'4+ N 0.41427 0.10288 0.22418
N'5+ N 0.34047 0.02039 0.40520
C6+ C 0.58019 0.06127 0.38879
N7+ N 0.59639 -0.02389 0.50789
O8+ O 0.66742 -0.11983 0.50245
O9+ O 0.53481 0.01718 0.59667
N10+ N 0.67256 0.00651 0.28566
O11+ O 0.63629 -0.09702 0.23935
O12+ O 0.76960 0.07038 0.26221
N13+ N 0.63043 0.20265 0.42449
O14+ O 0.57433 0.29501 0.37552
O15+ O 0.72206 0.20552 0.49587
H*16+ H 0.15283 0.01936 0.33866

#END

S46. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 5-(trinitromethyl)tetrazole (cocrystal form).
data_FTNM_DAG_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_

```
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 18.357
_cell_length_b                 8.771
_cell_length_c                 7.253
_cell_angle_alpha               90.00
_cell_angle_beta                99.04
_cell_angle_gamma                 90.00
_cell_volume                   1153.29
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.14692 0.10359 0.51826
N'2 N -0.09386 0.05532 0.43567
N3 N -0.15481 0.25955 0.54965
H*4 H -0.16880 0.28240 0.67660
N5 N -0.19872 0.01263 0.58577
N6 N -0.09872 0.36036 0.51091
N7 N -0.09803 -0.10706 0.40397
H*8 H -0.07101 -0.15963 0.52107
H*9 H -0.04966 0.30259 0.52969
H*10 H -0.10960 0.38485 0.37202
H*11 H -0.06651 -0.12718 0.30306
H*12 H -0.24864 0.06293 0.58243
H*13 H -0.20175 -0.09213 0.52470
C1+ C 0.56790 0.25640 0.06189
N2+ N 0.47042 0.31319 0.14458
N'3+ N 0.46083 0.34350 -0.03770
N'4+ N 0.52284 0.30740 -0.09273
N'5+ N 0.53605 0.25842 0.21417
C6+ C 0.64436 0.20350 0.05390
N7+ N 0.67745 0.11160 0.22920
O8+ O 0.69315 -0.02086 0.20831
O9+ O 0.68478 0.18559 0.37254
N10+ N 0.64413 0.10145 -0.12193
O11+ O 0.59733 0.00255 -0.13950
O12+ O 0.68963 0.12921 -0.22170
N13+ N 0.69966 0.33682 0.04000
O14+ O 0.67248 0.45646 -0.02032
O15+ O 0.76432 0.30620 0.08779
H*16+ H 0.43019 0.33051 0.22358

#END

data_FTNM_DAG_2
```

```
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.951
_cell_length_b                 12.759
_cell_length_c                 10.345
_cell_angle_alpha               90.00
_cell_angle_beta                104.47
_cell_angle_gamma                90.00
_cell_volume                   1143.98
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.77193 0.69618 0.41403
N'2 N 0.82520 0.69868 0.30892
N3 N 0.71394 0.60263 0.45235
H*4 H 0.61723 0.61326 0.48504
N5 N 0.76287 0.78100 0.49575
N6 N 0.69697 0.51512 0.36535
N7 N 0.88979 0.79969 0.29127
H*8 H 0.80217 0.84612 0.23886
H*9 H 0.67677 0.54210 0.26933
H*10 H 0.80145 0.47871 0.38392
H*11 H 0.95895 0.78684 0.22839
H*12 H 0.77342 0.76172 0.59271
H*13 H 0.83567 0.83937 0.48364
C1+ C 0.66394 0.06255 0.19267
N2+ N 0.52108 -0.03190 0.26596
N'3+ N 0.49027 0.06490 0.30028
N'4+ N 0.58081 0.12633 0.25375
N'5+ N 0.62819 -0.03810 0.19853
C6+ C 0.78061 0.10495 0.12624
N7+ N 0.82809 0.02407 0.03247
O8+ O 0.79954 0.04446 -0.08562
O9+ O 0.89198 -0.05291 0.09004
N10+ N 0.71359 0.20377 0.04347
O11+ O 0.58526 0.19136 -0.02858
O12+ O 0.79385 0.28158 0.05798
N13+ N 0.93410 0.13884 0.22664
O14+ O 0.92499 0.15824 0.33926
O15+ O 1.04623 0.14414 0.18101
H*16+ H 0.46595 -0.09588 0.28957
```

```
#END

data_FTNM_DAG_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 18.860
_cell_length_b                 10.760
_cell_length_c                 14.290
_cell_angle_alpha               90.00
_cell_angle_beta                55.95
_cell_angle_gamma                 90.00
_cell_volume                   2402.73
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.58407 0.68235 0.04903
N'2 N 0.53402 0.58728 0.07838
N3 N 0.56541 0.79212 0.01464
H*4 H 0.61813 0.83303 -0.05194
N5 N 0.65900 0.68683 0.04572
N6 N 0.49741 0.79182 -0.00087
N7 N 0.56041 0.48642 0.11882
H*8 H 0.60457 0.43463 0.05044
H*9 H 0.49195 0.70415 -0.02402
H*10 H 0.44240 0.80653 0.07638
H*11 H 0.50813 0.43069 0.16348
H*12 H 0.67275 0.77210 0.06177
H*13 H 0.66005 0.61848 0.09416
C1+ C 0.26127 0.09429 0.29420
N2+ N 0.14556 0.09666 0.31417
N'3+ N 0.20301 0.10187 0.20289
N'4+ N 0.27751 0.10020 0.18878
N'5+ N 0.17821 0.09157 0.37527
C6+ C 0.33153 0.09019 0.31250
N7+ N 0.29995 0.04845 0.43349
O8+ O 0.32843 -0.04753 0.44412
```

```
O9+ O 0.24899 0.11964 0.50652
N10+ N 0.40204 -0.00156 0.22631
O11+ O 0.37483 -0.10189 0.22156
O12+ O 0.47551 0.03463 0.17376
N13+ N 0.37553 0.21887 0.29573
O14+ O 0.36809 0.29336 0.23799
O15+ O 0.41401 0.23031 0.34052
H*16+ H 0.08160 0.09623 0.34915

#END

data_FTNM_DAG_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 8.855
_cell_length_b                 9.601
_cell_length_c                 14.208
_cell_angle_alpha               90.00
_cell_angle_beta               106.87
_cell_angle_gamma                90.00
_cell_volume                   1155.94
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.32351 0.22869 0.22533
N'2 N 0.20044 0.17359 0.24178
N3 N 0.38207 0.35574 0.26893
H*4 H 0.41772 0.41990 0.22282
N5 N 0.40633 0.17402 0.16455
N6 N 0.29317 0.43042 0.32074
N7 N 0.16506 0.03843 0.19635
H*8 H 0.09555 0.05308 0.12570
H*9 H 0.17622 0.40769 0.29001
H*10 H 0.32165 0.39032 0.39005
H*11 H 0.09403 -0.00864 0.23166
H*12 H 0.52310 0.19712 0.18590
H*13 H 0.38403 0.07049 0.15281
C1+ C 0.10982 0.72689 0.03322
N2+ N -0.04782 0.72403 0.11288
N'3+ N -0.10160 0.82124 0.04436
N'4+ N -0.00187 0.82408 -0.00739
```

```
N'5+ N 0.08344 0.66161 0.10937
C6+ C 0.24469 0.69928 -0.00681
N7+ N 0.32968 0.56077 0.03144
O8+ O 0.32823 0.47003 -0.02814
O9+ O 0.39147 0.55912 0.11978
N10+ N 0.18349 0.69376 -0.12118
O11+ O 0.06908 0.61952 -0.15289
O12+ O 0.25420 0.76184 -0.16660
N13+ N 0.37535 0.81390 0.02096
O14+ O 0.33357 0.92690 0.04244
O15+ O 0.50468 0.77882 0.01644
H*16+ H -0.10392 0.69965 0.16365

#END

data_FTNM_DAG_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 10.414
_cell_length_b                 18.681
_cell_length_c                 7.702
_cell_angle_alpha               90.00
_cell_angle_beta                55.15
_cell_angle_gamma                90.00
_cell_volume                   1229.64
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.19251 0.52286 0.10573
N'2 N 0.05717 0.49251 0.19704
N3 N 0.22714 0.58337 -0.02067
H*4 H 0.33779 0.58291 -0.15367
N5 N 0.31447 0.49999 0.11679
N6 N 0.11957 0.60498 -0.06761
N7 N 0.03960 0.43435 0.33228
H*8 H 0.08386 0.38913 0.24137
H*9 H 0.06210 0.56052 -0.06761
H*10 H 0.03644 0.63533 0.05632
H*11 H -0.07767 0.42579 0.43165
H*12 H 0.38413 0.54005 0.10678
H*13 H 0.27470 0.46740 0.24376
```

C1+ C -0.10440 0.12926 0.62772
N2+ N -0.27483 0.07403 0.63211
N'3+ N -0.15739 0.07890 0.42814
N'4+ N -0.04716 0.11408 0.42286
N'5+ N -0.24826 0.10435 0.76376
C6+ C -0.01043 0.16919 0.68576
N7+ N -0.07853 0.16264 0.92376
O8+ O 0.00096 0.13350 0.97187
O9+ O -0.20784 0.18890 1.03924
N10+ N 0.16021 0.13993 0.55409
O11+ O 0.16895 0.07519 0.55592
O12+ O 0.26547 0.18334 0.46514
N13+ N -0.00082 0.25126 0.64090
O14+ O -0.02452 0.26913 0.51004
O15+ O 0.03222 0.28863 0.73884
H*16+ H -0.37668 0.04872 0.68224

#END

S47. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 5-(trinitromethyl)tetrazole (cocrystal form).

data_FTNM_TAG_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.826
_cell_length_b 8.574
_cell_length_c 12.949
_cell_angle_alpha 90.00
_cell_angle_beta 90.32
_cell_angle_gamma 90.00
_cell_volume 1201.93
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.20651 0.57943 0.50619
N'2 N 0.15280 0.54431 0.59243
N3 N 0.23391 0.45756 0.66017
N4 N 0.33040 0.54718 0.48665
N5 N 0.36971 0.55738 0.38266
N6 N 0.14103 0.65417 0.42887
N7 N 0.02709 0.72591 0.45229

```
H*8 H 0.17800 0.41259 0.71553
H*9 H 0.29049 0.53493 0.69779
H*10 H 0.35857 0.45252 0.52833
H*11 H 0.45981 0.59033 0.38248
H*12 H 0.36124 0.45273 0.34585
H*13 H 0.19245 0.71245 0.37661
H*14 H -0.03734 0.63944 0.45620
H*15 H 0.03248 0.76977 0.52575
C1+ C 0.18324 0.47767 0.16722
N2+ N 0.04151 0.42461 0.26381
N'3+ N -0.00207 0.53801 0.20336
N'4+ N 0.08771 0.57304 0.14090
N'5+ N 0.15645 0.38208 0.24467
C6+ C 0.30329 0.48309 0.11192
N7+ N 0.38419 0.33800 0.13389
O8+ O 0.40885 0.25334 0.06192
O9+ O 0.41575 0.32577 0.22372
N10+ N 0.27859 0.49412 -0.00647
O11+ O 0.20486 0.39907 -0.03878
O12+ O 0.33408 0.59348 -0.05404
N13+ N 0.38471 0.62642 0.14252
O14+ O 0.32996 0.73680 0.17894
O15+ O 0.49420 0.61371 0.12495
H*16+ H -0.00998 0.37453 0.32004

#END

data_FTNM_TAG_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21'
_symmetry_Int_Tables_number      4
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,-z
_cell_length_a                  10.857
_cell_length_b                  10.232
_cell_length_c                  5.853
_cell_angle_alpha                 90.00
_cell_angle_beta                 107.73
_cell_angle_gamma                  90.00
_cell_volume                    619.32
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.22894 0.62911 0.99194
N'2 N 0.18181 0.68353 1.14736
N3 N 0.15770 0.82113 1.09921
```

N4 N 0.24368 0.69502 0.79348
N5 N 0.32317 0.63525 0.67109
N6 N 0.26573 0.49937 1.01709
N7 N 0.22334 0.41846 1.17382
H*8 H 0.14386 0.85834 1.25057
H*9 H 0.07071 0.83122 0.96825
H*10 H 0.25608 0.79262 0.82867
H*11 H 0.28929 0.66072 0.49531
H*12 H 0.41687 0.66515 0.73883
H*13 H 0.26999 0.45448 0.86584
H*14 H 0.28013 0.43900 1.34366
H*15 H 0.13244 0.44777 1.16938
C1+ C 0.18471 0.08236 0.58744
N2+ N 0.00981 0.09722 0.64638
N'3+ N 0.01092 -0.02206 0.55551
N'4+ N 0.12257 -0.03307 0.51720
N'5+ N 0.11568 0.16662 0.67069
C6+ C 0.31697 0.10668 0.57148
N7+ N 0.38229 0.22638 0.72122
O8+ O 0.47974 0.20787 0.88670
O9+ O 0.32717 0.32898 0.65220
N10+ N 0.40245 -0.01628 0.66213
O11+ O 0.39768 -0.05762 0.85356
O12+ O 0.46441 -0.05779 0.53692
N13+ N 0.31934 0.13463 0.31048
O14+ O 0.22731 0.09437 0.15083
O15+ O 0.41424 0.19171 0.29420
H*16+ H -0.06652 0.13178 0.69392

#END

data_FTNM_TAG_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 25.765
_cell_length_b 6.653
_cell_length_c 7.395
_cell_angle_alpha 90.00
_cell_angle_beta 91.72
_cell_angle_gamma 90.00
_cell_volume 1267.04
loop_
_atom_site_label
_atom_site_type_symbol

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.56505 0.50928 0.73273
N'2 N 0.54527 0.33778 0.68346
N3 N 0.58398 0.18073 0.68519
N4 N 0.61647 0.53184 0.79334
N5 N 0.63641 0.73027 0.80199
N6 N 0.53465 0.68031 0.72885
N7 N 0.48005 0.66157 0.71502
H*8 H 0.56723 0.06494 0.61528
H*9 H 0.58901 0.12985 0.81528
H*10 H 0.63922 0.42401 0.73784
H*11 H 0.66354 0.73663 0.90433
H*12 H 0.65318 0.76967 0.68392
H*13 H 0.54737 0.79433 0.80894
H*14 H 0.47072 0.63143 0.58285
H*15 H 0.46955 0.53502 0.78383
C1+ C 0.11684 0.46745 0.23394
N2+ N 0.05129 0.63632 0.25260
N'3+ N 0.05003 0.56677 0.08349
N'4+ N 0.09177 0.45793 0.06962
N'5+ N 0.09200 0.57900 0.35267
C6+ C 0.16664 0.35966 0.27096
N7+ N 0.18024 0.34388 0.47563
O8+ O 0.18265 0.17754 0.54227
O9+ O 0.18766 0.50552 0.54841
N10+ N 0.16287 0.14388 0.18988
O11+ O 0.12397 0.05317 0.22959
O12+ O 0.19824 0.08796 0.09776
N13+ N 0.21435 0.46421 0.18555
O14+ O 0.20459 0.57509 0.05872
O15+ O 0.25640 0.42089 0.25279
H*16+ H 0.02300 0.72600 0.30077

#END

data_FTNM_TAG_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 10.895
_cell_length_b                 15.641
_cell_length_c                 7.253
_cell_angle_alpha               90.00
```

```
_cell_angle_beta                 102.36
_cell_angle_gamma                 90.00
_cell_volume                    1207.33
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.32732 0.64629 0.04817
N'2 N 0.27901 0.71893 -0.01665
N3 N 0.16191 0.70749 -0.15182
N4 N 0.26681 0.56820 0.00241
N5 N 0.34063 0.49331 0.04538
N6 N 0.44339 0.64394 0.17058
N7 N 0.49463 0.71994 0.26070
H*8 H 0.14407 0.76496 -0.21755
H*9 H 0.09179 0.69895 -0.07937
H*10 H 0.20780 0.57155 -0.12720
H*11 H 0.28432 0.44562 0.07419
H*12 H 0.37902 0.47540 -0.06519
H*13 H 0.46137 0.59091 0.25156
H*14 H 0.53020 0.75398 0.16422
H*15 H 0.42238 0.75658 0.28708
C1+ C 0.75145 -0.01915 -0.00496
N2+ N 0.69244 0.10454 -0.03788
N'3+ N 0.60033 0.05917 -0.14452
N'4+ N 0.63674 -0.02028 -0.12457
N'5+ N 0.78893 0.05908 0.05262
C6+ C 0.82343 -0.09911 0.05285
N7+ N 0.93167 -0.08590 0.22712
O8+ O 0.92705 -0.12490 0.36991
O9+ O 1.01229 -0.03681 0.19953
N10+ N 0.73276 -0.16890 0.09963
O11+ O 0.66697 -0.14487 0.20493
O12+ O 0.73655 -0.23886 0.02901
N13+ N 0.88647 -0.13637 -0.10402
O14+ O 0.84022 -0.11452 -0.26439
O15+ O 0.97388 -0.18464 -0.04965
H*16+ H 0.68841 0.16911 -0.02676

#END

data_FTNM_TAG_5
_symmetry_cell_setting           monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.478
_cell_length_b 7.537
_cell_length_c 22.145
_cell_angle_alpha 90.00
_cell_angle_beta 77.14
_cell_angle_gamma 90.00
_cell_volume 1216.82
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.50939 0.26037 0.48603
N'2 N 0.42704 0.27982 0.44072
N3 N 0.23167 0.25249 0.46074
N4 N 0.41607 0.23106 0.54707
N5 N 0.52120 0.17104 0.58898
N6 N 0.69828 0.27067 0.47508
N7 N 0.79724 0.34464 0.41891
H*8 H 0.18589 0.23896 0.42106
H*9 H 0.17354 0.36735 0.48078
H*10 H 0.29422 0.16889 0.54813
H*11 H 0.46233 0.21766 0.63182
H*12 H 0.52530 0.03586 0.59034
H*13 H 0.75019 0.29944 0.51235
H*14 H 0.80447 0.24975 0.38564
H*15 H 0.71981 0.44405 0.40616
C1+ C 0.73385 0.26410 0.22441
N2+ N 0.56098 0.26720 0.30963
N'3+ N 0.45217 0.24794 0.26989
N'4+ N 0.56111 0.24542 0.21506
N'5+ N 0.73792 0.27769 0.28390
C6+ C 0.89737 0.26649 0.17192
N7+ N 1.07843 0.23803 0.19340
O8+ O 1.16802 0.10684 0.17513
O9+ O 1.11214 0.35524 0.22687
N10+ N 0.87788 0.11774 0.12498
O11+ O 0.83756 -0.02629 0.14859
O12+ O 0.90469 0.15842 0.07073
N13+ N 0.92200 0.44561 0.13551
O14+ O 0.78469 0.53508 0.14017
O15+ O 1.07543 0.47539 0.10536
H*16+ H 0.51143 0.27278 0.35613

#END

S48. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 5-nitrotetrazole 2*N*-oxide (cocrystal form).
data_T_2O_NH3_1

```
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 11.040
_cell_length_b                 8.782
_cell_length_c                 5.712
_cell_angle_alpha               90.00
_cell_angle_beta                76.13
_cell_angle_gamma               90.00
_cell_volume                   537.65
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.53064 0.23449 0.31400
H*2 H 0.46623 0.16756 0.26239
H*3 H 0.58252 0.16486 0.39432
H*4 H 0.58881 0.27484 0.16029
C1+ C 0.26302 0.07840 0.77642
N'2+ N 0.29131 0.00305 0.56633
N3+ N 0.17966 -0.00794 0.52922
N'4+ N 0.08702 0.05296 0.69518
N'5+ N 0.14132 0.10987 0.85807
O6+ O 0.16171 -0.07871 0.32940
H*7+ H 0.07207 -0.07167 0.34421
N8+ N 0.35799 0.12174 0.90349
O9+ O 0.32137 0.19016 1.09365
O10+ O 0.46563 0.08574 0.80832

#END

data_T_2O_NH3_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.960
```

```
_cell_length_b                  5.909
_cell_length_c                  12.285
_cell_angle_alpha                 90.00
_cell_angle_beta                 79.51
_cell_angle_gamma                   90.00
_cell_volume                    568.175
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.22989 0.68099 -0.02701
H*2 H 0.23427 0.58414 -0.09611
H*3 H 0.11356 0.75842 -0.01245
H*4 H 0.23232 0.57277 0.03728
C1+ C -0.23914 0.76337 0.26529
N'2+ N -0.29652 0.55791 0.24382
N3+ N -0.37734 0.50649 0.34276
N'4+ N -0.37461 0.65966 0.42162
N'5+ N -0.28392 0.82885 0.37113
O6+ O -0.45910 0.30525 0.36185
H*7+ H -0.50817 0.30836 0.44055
N8+ N -0.13651 0.90218 0.17956
O9+ O -0.09124 1.08672 0.20869
O10+ O -0.10504 0.82142 0.08633

#END

data_T_2O_NH3_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  10.939
_cell_length_b                  9.909
_cell_length_c                  5.070
_cell_angle_alpha                 90.00
_cell_angle_beta                106.88
_cell_angle_gamma                   90.00
_cell_volume                    525.883
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

```
_atom_site_fract_z
N1 N 0.33026 0.35902 -0.19076
H*2 H 0.39017 0.41346 -0.03584
H*3 H 0.27124 0.42632 -0.31858
H*4 H 0.38508 0.31627 -0.29999
C1+ C 0.58322 0.28336 0.44948
N'2+ N 0.47277 0.22575 0.45227
N3+ N 0.46406 0.13545 0.26072
N'4+ N 0.55781 0.13268 0.14282
N'5+ N 0.63639 0.22972 0.26616
O6+ O 0.36316 0.04983 0.18951
H*7+ H 0.37906 -0.00631 0.04502
N8+ N 0.63965 0.39520 0.63234
O9+ O 0.74064 0.43979 0.61170
O10+ O 0.58084 0.43423 0.78968

#END

data_T_2O_NH3_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.525
_cell_length_b                 13.068
_cell_length_c                 5.784
_cell_angle_alpha               90.00
_cell_angle_beta                93.17
_cell_angle_gamma               90.00
_cell_volume                   567.909
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.24087 0.39826 0.65717
H*2 H 0.11984 0.39889 0.56894
H*3 H 0.23003 0.44332 0.79950
H*4 H 0.26179 0.32541 0.71542
C1+ C 0.32352 0.11799 0.92005
N'2+ N 0.28717 0.17102 0.72482
N3+ N 0.16769 0.11045 0.62695
N'4+ N 0.12828 0.02643 0.74297
N'5+ N 0.23036 0.03101 0.93577
O6+ O 0.08963 0.13400 0.41688
```

H*7+ H 0.00724 0.07771 0.38301
N8+ N 0.45415 0.15311 1.09905
O9+ O 0.47639 0.09851 1.26978
O10+ O 0.52958 0.23397 1.06213

#END

data_T_2O_NH3_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 15.508
_cell_length_b 6.534
_cell_length_c 5.456
_cell_angle_alpha 90.00
_cell_angle_beta 91.91
_cell_angle_gamma 90.00
_cell_volume 552.545
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.52588 -0.14560 0.76519
H*2 H 0.57889 -0.06881 0.83143
H*3 H 0.47632 -0.04313 0.75686
H*4 H 0.53795 -0.18610 0.58927
C1+ C 0.21328 0.09932 0.77141
N'2+ N 0.14780 0.17887 0.63615
N3+ N 0.08436 0.12931 0.77529
N'4+ N 0.10482 0.02814 0.98035
N'5+ N 0.18949 0.00803 0.97868
O6+ O 0.00213 0.18050 0.70935
H*7+ H -0.03223 0.12709 0.84137
N8+ N 0.30273 0.11234 0.69656
O9+ O 0.35710 0.03433 0.83437
O10+ O 0.31523 0.20008 0.50279

#END

S49. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 5-nitrotetrazole 2*N*-oxide (cocrystal form).
data_T_2O_NH2OH_1
_symmetry_cell_setting monoclinic

```
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 15.927
_cell_length_b                 5.802
_cell_length_c                 13.904
_cell_angle_alpha               90.00
_cell_angle_beta               114.90
_cell_angle_gamma                90.00
_cell_volume                   1165.41
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.17238 0.15838 0.63098
H*2 H -0.15960 0.25620 0.57746
H*3 H -0.16876 0.26938 0.68969
O4 O -0.09021 0.01810 0.68033
H*5 H -0.11504 -0.13630 0.66929
C1+ C 0.63156 0.00906 0.09438
N'2+ N 0.59056 -0.18629 0.04580
N3+ N 0.57820 -0.28245 0.12358
N'4+ N 0.60750 -0.16530 0.21399
N'5+ N 0.64264 0.02646 0.19521
O6+ O 0.53724 -0.49197 0.11060
H*7+ H 0.53628 -0.52453 0.17891
N8+ N 0.66127 0.18646 0.04077
O9+ O 0.69790 0.35746 0.09289
O10+ O 0.64686 0.14809 -0.05143

#END

data_T_2O_NH2OH_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                5.331
_cell_length_b                12.978
_cell_length_c                17.360
_cell_angle_alpha              90.00
_cell_angle_beta               150.35
_cell_angle_gamma                90.00
_cell_volume                  594.167
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.21942 0.61262 -0.45806
H*2 H 0.02404 0.67915 -0.52078
H*3 H 0.06934 0.55886 -0.53462
O4 O 0.04278 0.58088 -0.43003
H*5 H 0.35396 0.57459 -0.31811
C1+ C -0.31361 0.05369 0.66622
N'2+ N -0.28616 0.09728 0.60369
N3+ N -0.51398 0.18403 0.55816
N'4+ N -0.67585 0.19723 0.58677
N'5+ N -0.54508 0.11177 0.65780
O6+ O -0.57736 0.25590 0.48542
H*7+ H -0.75411 0.31222 0.46392
N8+ N -0.10663 -0.04864 0.73719
O9+ O -0.15343 -0.08064 0.79053
O10+ O 0.09491 -0.09314 0.73689

#END

data_T_2O_NH2OH_3
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                10.375
_cell_length_b                10.808
_cell_length_c                5.375
_cell_angle_alpha              90.00
_cell_angle_beta               90.00
_cell_angle_gamma                90.00
_cell_volume                  602.715
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.30960 -0.13149 0.34234
H*2 H 0.30563 -0.08331 0.50581
H*3 H 0.39995 -0.11643 0.27282
O4 O 0.22649 -0.06234 0.17722
H*5 H 0.16603 -0.12433 0.12165
C1+ C 0.20547 0.35315 0.18649
N'2+ N 0.16700 0.45641 0.07012
N3+ N 0.04523 0.45368 0.12945
N'4+ N 0.00634 0.35949 0.26952
N'5+ N 0.11131 0.29313 0.30754
O6+ O -0.03558 0.54383 0.04950
H*7+ H -0.11926 0.52080 0.11773
N8+ N 0.33923 0.31084 0.18011
O9+ O 0.36320 0.21541 0.29298
O10+ O 0.41526 0.37465 0.06246

#END

data_T_2O_NH2OH_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 7.729
_cell_length_b                 4.625
_cell_length_c                 16.085
_cell_angle_alpha               90.00
_cell_angle_beta                95.15
_cell_angle_gamma                 90.00
_cell_volume                   572.663
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.18469 0.63593 0.48620
H*2 H 0.06361 0.72634 0.48313
H*3 H 0.23461 0.69151 0.43168
O4 O 0.15103 0.32953 0.47733
```

```
H*5 H 0.21476 0.25000 0.52641
C1+ C 0.67514 0.11984 0.35001
N'2+ N 0.55395 0.29949 0.31463
N3+ N 0.41827 0.19301 0.34635
N'4+ N 0.44513 -0.03218 0.39718
N'5+ N 0.61377 -0.08115 0.39980
O6+ O 0.25905 0.31072 0.32730
H*7+ H 0.18172 0.19420 0.35832
N8+ N 0.85826 0.14400 0.33493
O9+ O 0.95716 -0.03165 0.37054
O10+ O 0.89625 0.33772 0.28804

#END

data_T_2O_NH2OH_5
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 13.623
_cell_length_b                 7.301
_cell_length_c                 5.923
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   589.111
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.10959 0.19046 0.36668
H*2 H -0.05100 0.19529 0.25907
H*3 H -0.17034 0.20757 0.26760
O4 O -0.10289 0.36010 0.49161
H*5 H -0.10202 0.31873 0.64634
C1+ C 0.14857 0.25321 -0.00683
N'2+ N 0.17850 0.32672 -0.20239
N3+ N 0.09301 0.36139 -0.29145
N'4+ N 0.01467 0.31640 -0.16983
N'5+ N 0.05078 0.24523 0.01742
O6+ O 0.08656 0.43965 -0.49841
H*7+ H 0.01624 0.45077 -0.52559
N8+ N 0.21770 0.18791 0.16383
O9+ O 0.18203 0.12343 0.33569
```

O10+ O 0.30504 0.20358 0.11957

#END

S50. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 5-nitrotetrazole 2*N*-oxide (cocrystal form).

```
data_T_2O_N2H4_1
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                  12.595
_cell_length_b                  5.073
_cell_length_c                  7.714
_cell_angle_alpha                77.78
_cell_angle_beta                111.64
_cell_angle_gamma                137.84
_cell_volume                    306
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.30761 -0.30250 0.22427
H*2 H 0.42840 -0.15138 0.25482
H*3 H 0.27805 -0.21059 0.10423
N4 N 0.28530 -0.22315 0.36836
H*5 H 0.25745 -0.42289 0.46323
H*6 H 0.39139 0.05183 0.43728
C1+ C 0.24954 0.16807 0.78501
N'2+ N 0.17593 0.27529 0.68442
N3+ N 0.08559 0.15229 0.78617
N'4+ N 0.09714 -0.01793 0.93764
N'5+ N 0.20476 -0.00830 0.93753
O6+ O -0.01417 0.19967 0.73646
H*7+ H -0.06709 0.08547 0.83336
N8+ N 0.36838 0.23962 0.73100
O9+ O 0.42772 0.12917 0.83333
O10+ O 0.39790 0.40355 0.58829

#END

data_T_2O_N2H4_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
```

```
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 11.443
_cell_length_b                 9.938
_cell_length_c                 5.552
_cell_angle_alpha               90.00
_cell_angle_beta                82.28
_cell_angle_gamma                 90.00
_cell_volume                   625.654
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.19839 0.32567 0.25953
H*2 H 0.22950 0.41495 0.18622
H*3 H 0.12858 0.29797 0.17516
N4 N 0.15721 0.33714 0.51477
H*5 H 0.22679 0.31836 0.60604
H*6 H 0.12705 0.43153 0.56079
C1+ C -0.42510 0.77064 0.07481
N'2+ N -0.52292 0.70353 0.03929
N3+ N -0.52479 0.61543 0.21365
N'4+ N -0.43824 0.62249 0.35057
N'5+ N -0.37246 0.72436 0.26005
O6+ O -0.61191 0.52227 0.24934
H*7+ H -0.59344 0.46971 0.38758
N8+ N -0.38074 0.88451 -0.07729
O9+ O -0.29074 0.93805 -0.02808
O10+ O -0.43757 0.91609 -0.24021

#END

data_T_2O_N2H4_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 5.967
_cell_length_b                 7.792
_cell_length_c                 13.794
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 71.73
_cell_angle_gamma                90.00
_cell_volume                    609.02
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.28083 0.82614 -0.08060
H*2 H 0.36292 0.92434 -0.12716
H*3 H 0.13065 0.79761 -0.09722
N4 N 0.21404 0.87301 0.02538
H*5 H 0.35174 0.84424 0.05108
H*6 H 0.18125 1.00127 0.03603
C1+ C 0.23437 0.24346 0.78301
N'2+ N 0.32221 0.09427 0.73894
N3+ N 0.25756 0.10524 0.65724
N'4+ N 0.13988 0.24558 0.64751
N'5+ N 0.12416 0.33686 0.72999
O6+ O 0.31027 -0.02231 0.58690
H*7+ H 0.24385 0.01625 0.53446
N8+ N 0.25827 0.29784 0.88070
O9+ O 0.17120 0.43640 0.91361
O10+ O 0.36321 0.19992 0.92082

#END

data_T_2O_N2H4_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  9.954
_cell_length_b                  8.724
_cell_length_c                  8.190
_cell_angle_alpha                90.00
_cell_angle_beta                 63.56
_cell_angle_gamma                90.00
_cell_volume                    636.817
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

```
_atom_site_fract_z
N1 N 0.29203 0.03918 0.18402
H*2 H 0.39951 0.03136 0.16788
H*3 H 0.26117 -0.06619 0.15965
N4 N 0.27930 0.14426 0.05656
H*5 H 0.25847 0.24995 0.11498
H*6 H 0.37612 0.15080 -0.06190
C1+ C 0.26623 0.60462 0.15439
N'2+ N 0.19275 0.72535 0.13215
N3+ N 0.09552 0.65244 0.09476
N'4+ N 0.10280 0.50030 0.09217
N'5+ N 0.21483 0.46828 0.13127
O6+ O -0.00677 0.73102 0.06074
H*7+ H -0.06489 0.65171 0.03717
N8+ N 0.39163 0.62216 0.19999
O9+ O 0.45019 0.50399 0.21696
O10+ O 0.42682 0.75344 0.21711

#END

data_T_2O_N2H4_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 9.863
_cell_length_b                 13.180
_cell_length_c                 4.986
_cell_angle_alpha               90.00
_cell_angle_beta                84.29
_cell_angle_gamma                 90.00
_cell_volume                   644.936
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.22693 -0.13549 -0.59998
H*2 H -0.27899 -0.13992 -0.41303
H*3 H -0.29457 -0.14726 -0.73798
N4 N -0.12336 -0.21215 -0.64074
H*5 H -0.03635 -0.18314 -0.57803
H*6 H -0.14789 -0.27584 -0.53017
C1+ C -0.16263 0.60196 -0.06838
N'2+ N -0.23435 0.62678 -0.27338
```

N3+ N -0.34832 0.58106 -0.19254
N'4+ N -0.35271 0.53127 0.03992
N'5+ N -0.23090 0.54477 0.12237
O6+ O -0.45550 0.58540 -0.34249
H*7+ H -0.52656 0.54601 -0.24009
N8+ N -0.02191 0.63509 -0.05687
O9+ O 0.03345 0.60790 0.13973
O10+ O 0.02794 0.68705 -0.24487

#END

S51. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 5-nitrotetrazole 2*N*-oxide (cocrystal form).

data_T_2O_G_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 4.676
_cell_length_b 23.679
_cell_length_c 9.600
_cell_angle_alpha 90.00
_cell_angle_beta 43.10
_cell_angle_gamma 90.00
_cell_volume 726.28
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.30978 0.38080 0.81037
N'2 N 0.26899 0.32687 0.83063
H*3 H 0.24945 0.31312 0.93811
N4 N 0.38852 0.40739 0.65548
H*5 H 0.23383 0.44430 0.69588
H*6 H 0.36081 0.38051 0.58375
N7 N 0.28090 0.41913 0.93111
H*8 H 0.27965 0.40108 1.02706
H*9 H 0.47586 0.45282 0.85551
C1+ C 0.31558 0.11487 0.79984
N'2+ N 0.27193 0.14223 0.69403
N3+ N 0.26514 0.19389 0.74327
N'4+ N 0.30017 0.20049 0.86779
N'5+ N 0.33341 0.14867 0.90543
O6+ O 0.22398 0.23792 0.66877

H*7+ H 0.22774 0.27118 0.72727
N8+ N 0.34109 0.05332 0.79856
O9+ O 0.38069 0.03297 0.90074
O10+ O 0.32057 0.02766 0.69541

#END

data_T_2O_G_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 14.638
_cell_length_b 10.856
_cell_length_c 4.961
_cell_angle_alpha 90.00
_cell_angle_beta 111.42
_cell_angle_gamma 90.00
_cell_volume 733.9
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.37587 0.21300 0.36156
N'2 N 0.31904 0.14276 0.16224
H*3 H 0.29410 0.18627 -0.03361
N4 N 0.40902 0.17601 0.65053
H*5 H 0.48002 0.19691 0.76731
H*6 H 0.39215 0.08693 0.67187
N7 N 0.41217 0.32868 0.32649
H*8 H 0.37972 0.36553 0.12681
H*9 H 0.41939 0.38984 0.48742
C1+ C -0.12179 0.78620 0.70527
N'2+ N -0.17579 0.77485 0.42267
N3+ N -0.17109 0.65567 0.39881
N'4+ N -0.11985 0.59402 0.63773
N'5+ N -0.08729 0.67940 0.83981
O6+ O -0.21697 0.59981 0.14006
H*7+ H -0.20246 0.51256 0.17955
N8+ N -0.10282 0.90566 0.85115
O9+ O -0.05259 0.90487 1.10939
O10+ O -0.13886 0.99577 0.70197

#END

```
data_T_2O_G_3
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 23.810
_cell_length_b                 9.361
_cell_length_c                 6.618
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   1475.06
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.36946 0.48220 -0.23420
N'2 N 0.42334 0.47590 -0.23901
H*3 H 0.43690 0.37599 -0.27671
N4 N 0.34255 0.60484 -0.16405
H*5 H 0.30786 0.63369 -0.24288
H*6 H 0.36975 0.68667 -0.14246
N7 N 0.33150 0.37657 -0.29513
H*8 H 0.34912 0.28000 -0.32133
H*9 H 0.29585 0.37030 -0.21181
C1+ C 0.13483 0.49191 -0.22810
N'2+ N 0.10766 0.61236 -0.27735
N3+ N 0.05619 0.56632 -0.26118
N'4+ N 0.04953 0.43062 -0.20731
N'5+ N 0.10110 0.38122 -0.18537
O6+ O 0.01240 0.65499 -0.29846
H*7+ H -0.02075 0.59593 -0.27631
N8+ N 0.19611 0.48375 -0.22221
O9+ O 0.21629 0.36837 -0.17529
O10+ O 0.22173 0.59303 -0.26472

#END

data_T_2O_G_4
```

```
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 13.819
_cell_length_b                 24.061
_cell_length_c                 6.918
_cell_angle_alpha               90.00
_cell_angle_beta                39.91
_cell_angle_gamma                 90.00
_cell_volume                   1475.79
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.73288 0.87927 0.77746
N'2 N 0.72397 0.82599 0.79551
H*3 H 0.62455 0.81238 0.89055
N4 N 0.85226 0.90650 0.68530
H*5 H 0.89478 0.93937 0.54645
H*6 H 0.93279 0.87966 0.60757
N7 N 0.63355 0.91620 0.83911
H*8 H 0.53582 0.89875 0.94396
H*9 H 0.61781 0.95279 0.93301
C1+ C 0.24621 0.11593 0.74943
N'2+ N 0.37080 0.14374 0.61029
N3+ N 0.31993 0.19431 0.67046
N'4+ N 0.17760 0.19985 0.83142
N'5+ N 0.12863 0.14845 0.88391
O6+ O 0.41039 0.23832 0.57072
H*7+ H 0.34685 0.27066 0.64419
N8+ N 0.24089 0.05524 0.75215
O9+ O 0.12124 0.03437 0.88608
O10+ O 0.35655 0.03073 0.62025

#END

data_T_2O_G_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
```

```
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   6.957
_cell_length_b                   23.672
_cell_length_c                   4.665
_cell_angle_alpha                 90.00
_cell_angle_beta                 70.63
_cell_angle_gamma                   90.00
_cell_volume                     724.774
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.21268 -0.11755 -0.37081
N'2 N -0.19739 -0.17114 -0.34063
H*3 H -0.29365 -0.18485 -0.13594
N4 N -0.07824 -0.08948 -0.61968
H*5 H -0.14232 -0.05898 -0.71104
H*6 H 0.00945 -0.11668 -0.77666
N7 N -0.35597 -0.08109 -0.17721
H*8 H -0.43807 -0.09836 0.02464
H*9 H -0.30343 -0.04191 -0.15580
C1+ C -0.20470 0.61423 -0.39726
N'2+ N -0.09145 0.64325 -0.64160
N3+ N -0.12444 0.69413 -0.52905
N'4+ N -0.24583 0.69877 -0.24223
N'5+ N -0.29901 0.64638 -0.15455
O6+ O -0.03711 0.73932 -0.70155
H*7+ H -0.08491 0.77165 -0.56734
N8+ N -0.22227 0.55272 -0.39911
O9+ O -0.32979 0.53077 -0.16326
O10+ O -0.12789 0.52867 -0.63634

#END
```

S52. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 5-nitrotetrazole 2*N*-oxide (cocrystal form).

```
data_T_2O_AG_1
_symmetry_cell_setting           orthorhombic
_symmetry_space_group_name_H-M   'P n a 21'
_symmetry_Int_Tables_number      33
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.341
_cell_length_b 10.688
_cell_length_c 6.882
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 760.63
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.73532 0.62765 -0.17356
N2 N 0.64611 0.69748 -0.28008
H*3 H 0.56133 0.65231 -0.30434
N'4 N 0.85486 0.62508 -0.22883
N5 N 0.68458 0.56576 -0.01414
H*6 H 0.61024 0.61086 0.05137
H*7 H 0.75592 0.53815 0.07829
N8 N 0.93559 0.55978 -0.08978
H*9 H 0.94743 0.47063 -0.14077
H*10 H 1.02452 0.59993 -0.10206
H*11 H 0.68550 0.73081 -0.40475
C1+ C 0.17334 0.13771 0.59556
N'2+ N 0.06177 0.18161 0.66741
N3+ N 0.10644 0.23714 0.82209
N'4+ N 0.23337 0.23124 0.85088
N'5+ N 0.27780 0.16598 0.70238
O6+ O 0.02508 0.29727 0.94504
H*7+ H 0.08132 0.33007 1.04665
N8+ N 0.17896 0.06525 0.41566
O9+ O 0.28603 0.03002 0.36402
O10+ O 0.07609 0.04631 0.33281

#END

data_T_2O_AG_2
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 8.715
_cell_length_b 14.403

```
_cell_length_c                 8.177
_cell_angle_alpha               103.92
_cell_angle_beta                62.07
_cell_angle_gamma                152.28
_cell_volume                   382.112
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.13533 0.61478 -0.26415
N2 N -0.08679 0.62402 -0.11695
H*3 H -0.33279 0.47474 -0.00160
N'4 N -0.00944 0.75621 -0.33146
N5 N -0.32135 0.44845 -0.32461
H*6 H -0.26426 0.41090 -0.32291
H*7 H -0.27684 0.47616 -0.45784
N8 N -0.04445 0.73728 -0.49862
H*9 H -0.30230 0.64493 -0.43794
H*10 H 0.17966 0.89148 -0.58649
H*11 H 0.01517 0.73432 -0.06425
C1+ C 0.40725 0.15460 0.16391
N'2+ N 0.47812 0.22298 0.00653
N3+ N 0.35515 0.08836 -0.07305
N'4+ N 0.21752 -0.05405 0.02007
N'5+ N 0.25112 -0.01119 0.17593
O6+ O 0.37044 0.09697 -0.24265
H*7+ H 0.26364 -0.01807 -0.27047
N8+ N 0.49459 0.25421 0.30886
O9+ O 0.41765 0.17847 0.44642
O10+ O 0.63682 0.40442 0.27965

#END

data_T_2O_AG_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 4.512
_cell_length_b                 15.504
_cell_length_c                 11.366
_cell_angle_alpha               90.00
_cell_angle_beta                96.52
_cell_angle_gamma                90.00
```

```
_cell_volume                    789.955
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.61533 -0.13073 0.24660
N2 N 0.54243 -0.05381 0.30009
H*3 H 0.52531 -0.05947 0.38800
N'4 N 0.47335 -0.15211 0.14551
N5 N 0.83992 -0.17805 0.30989
H*6 H 0.99704 -0.14191 0.35792
H*7 H 0.92398 -0.22306 0.25756
N8 N 0.60038 -0.22852 0.09755
H*9 H 0.47209 -0.27964 0.11775
H*10 H 0.55944 -0.22219 0.00800
H*11 H 0.35883 -0.02604 0.25592
C1+ C 0.91654 0.10906 0.28468
N'2+ N 1.06835 0.07315 0.20254
N3+ N 0.91667 0.10489 0.10796
N'4+ N 0.68920 0.15620 0.12460
N'5+ N 0.68815 0.15916 0.24062
O6+ O 0.99240 0.08537 -0.00096
H*7+ H 0.84759 0.11652 -0.05533
N8+ N 0.99624 0.09419 0.41130
O9+ O 0.84199 0.13029 0.47810
O10+ O 1.21009 0.04697 0.43918

#END

data_T_2O_AG_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  7.610
_cell_length_b                  12.196
_cell_length_c                  8.441
_cell_angle_alpha                 90.00
_cell_angle_beta                 86.23
_cell_angle_gamma                   90.00
_cell_volume                    781.727
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.45843 0.37768 0.37027
N2 N 0.43771 0.36061 0.53383
H*3 H 0.34034 0.40624 0.58891
N'4 N 0.61527 0.38890 0.30338
N5 N 0.30303 0.38131 0.29385
H*6 H 0.20607 0.33266 0.34275
H*7 H 0.32628 0.37163 0.17454
N8 N 0.61253 0.39369 0.13201
H*9 H 0.61806 0.47476 0.10105
H*10 H 0.73039 0.36211 0.08997
H*11 H 0.55347 0.36914 0.58568
C1+ C 0.48910 0.12684 0.81572
N'2+ N 0.56419 0.11781 0.66818
N3+ N 0.42269 0.12153 0.58931
N'4+ N 0.27013 0.13187 0.67404
N'5+ N 0.31305 0.13539 0.82294
O6+ O 0.43458 0.11499 0.42868
H*7+ H 0.31301 0.11962 0.39940
N8+ N 0.59240 0.12719 0.95570
O9+ O 0.50984 0.13587 1.08426
O10+ O 0.75220 0.11878 0.93178

#END

data_T_2O_AG_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 6.900
_cell_length_b                 11.108
_cell_length_c                 11.511
_cell_angle_alpha               90.00
_cell_angle_beta                62.47
_cell_angle_gamma                 90.00
_cell_volume                   782.363
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.25580 0.27815 0.52663
```

N2 N -0.31801 0.18069 0.47498
H*3 H -0.46850 0.18967 0.48071
N'4 N -0.16544 0.25828 0.60136
N5 N -0.29959 0.39020 0.49149
H*6 H -0.28959 0.39349 0.40091
H*7 H -0.21336 0.45577 0.50898
N8 N -0.09030 0.36899 0.63382
H*9 H -0.20758 0.39459 0.72461
H*10 H 0.04029 0.34480 0.64725
H*11 H -0.30161 0.10158 0.51361
C1+ C 0.28643 0.21232 0.32300
N'2+ N 0.19900 0.14576 0.26198
N3+ N 0.19550 0.04182 0.31546
N'4+ N 0.27176 0.03885 0.40239
N'5+ N 0.33175 0.15071 0.40771
O6+ O 0.11693 -0.05695 0.28213
H*7+ H 0.13207 -0.12152 0.33472
N8+ N 0.32784 0.34117 0.29816
O9+ O 0.40810 0.39271 0.35947
O10+ O 0.27852 0.38594 0.21829

#END

S53. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 5-nitrotetrazole 2*N*-oxide (cocrystal form).

data_T_2O_DAG_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 9.725
_cell_length_b 19.977
_cell_length_c 4.795
_cell_angle_alpha 90.00
_cell_angle_beta 108.74
_cell_angle_gamma 90.00
_cell_volume 882.17
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.87475 -0.39344 -0.42907
N'2 N -0.94715 -0.37512 -0.69413
N3 N -0.73013 -0.37364 -0.30255

H*4 H -0.66615 -0.41050 -0.18315
N5 N -0.92670 -0.43371 -0.24917
N6 N -0.66005 -0.34069 -0.48170
N7 N -1.09676 -0.39627 -0.77766
H*8 H -1.10275 -0.44378 -0.86071
H*9 H -0.70547 -0.35703 -0.69388
H*10 H -0.68640 -0.29127 -0.48500
H*11 H -1.15031 -0.36699 -0.95234
H*12 H -0.88232 -0.42381 -0.03117
H*13 H -1.03720 -0.43424 -0.31878
C1+ C -0.34396 0.61095 -0.54948
N'2+ N -0.43219 0.63822 -0.79800
N3+ N -0.40395 0.70119 -0.73361
N'4+ N -0.30784 0.71470 -0.47207
N'5+ N -0.26807 0.65555 -0.35015
O6+ O -0.47101 0.74950 -0.92833
H*7+ H -0.43186 0.79127 -0.82946
N8+ N -0.33271 0.53857 -0.50323
O9+ O -0.24871 0.51938 -0.26807
O10+ O -0.40830 0.50366 -0.70380

#END

data_T_2O_DAG_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 17.506
_cell_length_b 10.904
_cell_length_c 4.897
_cell_angle_alpha 90.00
_cell_angle_beta 100.48
_cell_angle_gamma 90.00
_cell_volume 919.173
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.14362 0.26415 0.05725
N'2 N 0.10541 0.24794 0.25664
N3 N 0.21585 0.20789 0.06784
H*4 H 0.25510 0.26323 0.00029
N5 N 0.12025 0.33687 -0.17560

N6 N 0.25028 0.14629 0.31478
N7 N 0.03008 0.30581 0.19890
H*8 H 0.03671 0.39486 0.26509
H*9 H 0.23204 0.18781 0.47912
H*10 H 0.22723 0.06028 0.30475
H*11 H -0.00135 0.26475 0.32870
H*12 H 0.13901 0.30691 -0.34798
H*13 H 0.06200 0.35265 -0.20722
C1+ C -0.10986 0.24614 0.70182
N'2+ N -0.06845 0.17433 0.56099
N3+ N -0.09909 0.06874 0.60412
N'4+ N -0.15466 0.06949 0.75634
N'5+ N -0.16196 0.18588 0.82108
O6+ O -0.07430 -0.03529 0.49634
H*7+ H -0.10573 -0.10003 0.55736
N8+ N -0.09843 0.37884 0.72164
O9+ O -0.13949 0.43507 0.85552
O10+ O -0.04884 0.42183 0.60258

#END

data_T_2O_DAG_3
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P c a 21'
_symmetry_Int_Tables_number 29
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.352
_cell_length_b 7.042
_cell_length_c 16.776
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 868.54
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.38461 0.31148 0.38772
N'2 N 0.31921 0.23977 0.45257
N3 N 0.32911 0.24118 0.31369
H*4 H 0.43280 0.23053 0.27408
N5 N 0.51303 0.45559 0.38336
N6 N 0.21884 0.07598 0.31146
N7 N 0.38246 0.33974 0.52233

H*8 H 0.50384 0.28080 0.53908
H*9 H 0.24886 -0.00560 0.36023
H*10 H 0.08787 0.11923 0.31937
H*11 H 0.29353 0.30473 0.56639
H*12 H 0.50096 0.53932 0.33447
H*13 H 0.51843 0.53024 0.43525
C1+ C 0.71693 0.24774 0.14777
N'2+ N 0.74667 0.21847 0.06992
N3+ N 0.57865 0.19988 0.04641
N'4+ N 0.45075 0.21491 0.10203
N'5+ N 0.54093 0.24637 0.16876
O6+ O 0.54029 0.16689 -0.03138
H*7+ H 0.40800 0.15887 -0.03323
N8+ N 0.86545 0.27833 0.20423
O9+ O 0.82218 0.30355 0.27378
O10+ O 1.01976 0.27599 0.17690

#END

data_T_2O_DAG_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 12.021
_cell_length_b 13.865
_cell_length_c 6.507
_cell_angle_alpha 90.00
_cell_angle_beta 125.79
_cell_angle_gamma 90.00
_cell_volume 879.733
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.33885 0.60918 0.35182
N'2 N 0.22579 0.61926 0.33105
N3 N 0.46458 0.62704 0.58361
H*4 H 0.53193 0.66217 0.56419
N5 N 0.34948 0.58299 0.15804
N6 N 0.46464 0.66766 0.78373
N7 N 0.10814 0.59093 0.08380
H*8 H 0.07728 0.64955 -0.03321
H*9 H 0.37855 0.70927 0.70660

H*10 H 0.45276 0.61214 0.87186
H*11 H 0.03188 0.57944 0.10524
H*12 H 0.43575 0.54546 0.21691
H*13 H 0.26216 0.55017 0.01420
C1+ C 0.18555 0.11370 0.11360
N'2+ N 0.08073 0.17348 -0.03863
N3+ N 0.00259 0.15175 0.03275
N'4+ N 0.04946 0.08508 0.21220
N'5+ N 0.16970 0.05983 0.26602
O6+ O -0.12004 0.19619 -0.07425
H*7+ H -0.15745 0.16772 0.01031
N8+ N 0.30624 0.10856 0.11125
O9+ O 0.39549 0.05141 0.25831
O10+ O 0.30722 0.16188 -0.03757

#END

data_T_2O_DAG_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 10.552
_cell_length_b 11.207
_cell_length_c 8.229
_cell_angle_alpha 90.00
_cell_angle_beta 63.80
_cell_angle_gamma 90.00
_cell_volume 873.15
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.53211 0.84220 0.57306
N'2 N -0.58762 0.83606 0.46126
N3 N -0.60424 0.89983 0.73963
H*4 H -0.53978 0.94956 0.77455
N5 N -0.40086 0.79751 0.54283
N6 N -0.72948 0.96361 0.77314
N7 N -0.50245 0.76601 0.30334
H*8 H -0.42895 0.82153 0.21073
H*9 H -0.72216 0.99418 0.65206
H*10 H -0.80993 0.90327 0.81801
H*11 H -0.56823 0.74307 0.24798

H*12 H -0.39475 0.77036 0.65671
H*13 H -0.36727 0.73473 0.44324
C1+ C -0.18462 -0.11430 0.88849
N'2+ N -0.11268 -0.05143 0.73668
N3+ N -0.21881 -0.00973 0.71340
N'4+ N -0.34724 -0.04097 0.83544
N'5+ N -0.32535 -0.10971 0.95083
O6+ O -0.19610 0.06183 0.57037
H*7+ H -0.29047 0.08038 0.58373
N8+ N -0.11392 -0.18172 0.97692
O9+ O -0.19025 -0.23575 1.11465
O10+ O 0.01525 -0.17810 0.90528

#END

S54. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 5-nitrotetrazole 2*N*-oxide (cocrystal form).
data_T_2O_TAG_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 7.227
_cell_length_b 20.113
_cell_length_c 6.718
_cell_angle_alpha 90.00
_cell_angle_beta 66.43
_cell_angle_gamma 90.00
_cell_volume 895.038
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.48691 -0.10702 0.22266
N'2 N 0.43358 -0.04508 0.25736
N3 N 0.24468 -0.03304 0.23760
N4 N 0.36614 -0.15592 0.18838
N5 N 0.45972 -0.21744 0.10266
N6 N 0.66994 -0.12738 0.22127
N7 N 0.77473 -0.08531 0.30917
H*8 H 0.23518 0.01722 0.22855
H*9 H 0.12926 -0.04636 0.38055
H*10 H 0.27455 -0.13552 0.12205
H*11 H 0.35442 -0.25391 0.16013

H*12 H 0.51658 -0.21751 -0.06289
H*13 H 0.68091 -0.17635 0.24867
H*14 H 0.84340 -0.04959 0.19592
H*15 H 0.67076 -0.06017 0.43797
C1+ C 0.95926 0.15246 0.28342
N'2+ N 0.77711 0.15984 0.27784
N3+ N 0.74023 0.09782 0.25084
N'4+ N 0.88127 0.05383 0.23958
N'5+ N 1.02557 0.08949 0.26091
O6+ O 0.56518 0.08048 0.23553
H*7+ H 0.57448 0.03238 0.21638
N8+ N 1.07395 0.20885 0.31179
O9+ O 1.23837 0.19619 0.31439
O10+ O 0.99528 0.26366 0.33040

#END

data_T_2O_TAG_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 8.456
_cell_length_b 10.413
_cell_length_c 12.150
_cell_angle_alpha 90.00
_cell_angle_beta 116.40
_cell_angle_gamma 90.00
_cell_volume 958.264
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.50014 0.40947 0.62476
N'2 N 0.52862 0.48482 0.71673
N3 N 0.71504 0.50058 0.79535
N4 N 0.63507 0.35952 0.60129
N5 N 0.59083 0.25613 0.51693
N6 N 0.32951 0.37648 0.54351
N7 N 0.18690 0.44822 0.54225
H*8 H 0.72250 0.54067 0.87381
H*9 H 0.76307 0.56873 0.75729
H*10 H 0.74881 0.35182 0.68100
H*11 H 0.66938 0.26109 0.47363

H*12 H 0.60972 0.16980 0.56064
H*13 H 0.31245 0.34646 0.45983
H*14 H 0.16768 0.41797 0.61519
H*15 H 0.22607 0.54200 0.56150
C1+ C -0.05787 0.65830 0.10847
N'2+ N -0.19640 0.57947 0.05360
N3+ N -0.24339 0.57002 0.14194
N'4+ N -0.14754 0.63499 0.24435
N'5+ N -0.02542 0.69318 0.22283
O6+ O -0.38381 0.49677 0.12746
H*7+ H -0.39097 0.50568 0.20498
N8+ N 0.04756 0.70168 0.04746
O9+ O 0.17082 0.77346 0.10638
O10+ O 0.00312 0.66234 -0.05707

#END

data_T_2O_TAG_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 5.374
_cell_length_b 19.362
_cell_length_c 10.290
_cell_angle_alpha 90.00
_cell_angle_beta 63.64
_cell_angle_gamma 90.00
_cell_volume 959.361
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.70644 0.36902 0.29049
N'2 N 0.60215 0.35741 0.20051
N3 N 0.66063 0.28806 0.14314
N4 N 0.83812 0.31827 0.33366
N5 N 0.99834 0.34085 0.40393
N6 N 0.68666 0.43396 0.34987
N7 N 0.49714 0.48225 0.34160
H*8 H 0.61606 0.28821 0.05691
H*9 H 0.51876 0.25534 0.21739
H*10 H 0.92332 0.28171 0.25465
H*11 H 0.99225 0.30356 0.47468

H*12 H 1.19978 0.34941 0.33118
H*13 H 0.70549 0.43580 0.44329
H*14 H 0.58579 0.50201 0.23911
H*15 H 0.32593 0.45594 0.34911
C1+ C -0.20879 0.63541 0.16892
N'2+ N -0.18433 0.57934 0.08775
N3+ N -0.32226 0.60110 0.01873
N'4+ N -0.42729 0.66446 0.04991
N'5+ N -0.35329 0.68724 0.14858
O6+ O -0.35371 0.55995 -0.07950
H*7+ H -0.46231 0.58769 -0.11486
N8+ N -0.08689 0.63890 0.27056
O9+ O -0.12245 0.69263 0.33888
O10+ O 0.03981 0.58777 0.27824

#END

data_T_2O_TAG_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 9.770
_cell_length_b 11.340
_cell_length_c 9.230
_cell_angle_alpha 90.00
_cell_angle_beta 114.18
_cell_angle_gamma 90.00
_cell_volume 932.888
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.02167 0.62176 0.71008
N'2 N 0.07607 0.54108 0.72054
N3 N 0.10121 0.46189 0.85154
N4 N -0.10013 0.62407 0.80669
N5 N -0.17582 0.73012 0.80934
N6 N -0.05370 0.71006 0.59787
N7 N -0.00942 0.69673 0.47101
H*8 H 0.19615 0.41688 0.86686
H*9 H 0.01721 0.40024 0.81574
H*10 H -0.03883 0.58453 0.91299
H*11 H -0.26774 0.70936 0.82929

H*12 H -0.10869 0.78523 0.89697
H*13 H -0.15355 0.75086 0.56815
H*14 H 0.10242 0.71519 0.51472
H*15 H -0.01742 0.60930 0.44082
C1+ C 0.09656 0.10845 0.80066
N'2+ N 0.02070 0.04026 0.67451
N3+ N -0.09857 0.02052 0.70082
N'4+ N -0.10245 0.06975 0.82975
N'5+ N 0.02556 0.12765 0.89580
O6+ O -0.21144 -0.04729 0.59952
H*7+ H -0.28565 -0.04826 0.64492
N8+ N 0.24418 0.15709 0.83026
O9+ O 0.30285 0.21808 0.94904
O10+ O 0.29587 0.13246 0.73362

#END

data_T_2O_TAG_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 20.137
_cell_length_b 7.221
_cell_length_c 6.723
_cell_angle_alpha 90.00
_cell_angle_beta 83.08
_cell_angle_gamma 90.00
_cell_volume 970.465
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.64912 0.25531 0.45260
N'2 N 0.59647 0.30157 0.57288
N3 N 0.59465 0.20980 0.76429
N4 N 0.69966 0.14254 0.51013
N5 N 0.74576 0.06755 0.35509
N6 N 0.65754 0.32030 0.25797
N7 N 0.61838 0.47067 0.20495
H*8 H 0.54719 0.22811 0.83205
H*9 H 0.62459 0.28174 0.85004
H*10 H 0.68082 0.05545 0.62249
H*11 H 0.79053 0.05222 0.40838

H*12 H 0.73017 -0.05819 0.30951
H*13 H 0.70507 0.32005 0.18950
H*14 H 0.57228 0.41922 0.18757
H*15 H 0.61036 0.55811 0.32540
C1+ C 0.09870 0.69622 -0.09939
N'2+ N 0.10845 0.71773 -0.29876
N3+ N 0.04799 0.76558 -0.32820
N'4+ N 0.00282 0.77513 -0.16723
N'5+ N 0.03591 0.72966 -0.01643
O6+ O 0.03334 0.80298 -0.51560
H*7+ H -0.01406 0.83456 -0.49721
N8+ N 0.15256 0.64087 0.01564
O9+ O 0.13787 0.62556 0.19664
O10+ O 0.20752 0.61481 -0.07937

#END

S55. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 5-(trinitromethyl)tetrazole 2*N*-oxide (cocrystal form).
data_FTNM_2O_NH3_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 17.284
_cell_length_b 10.057
_cell_length_c 11.199
_cell_angle_alpha 90.00
_cell_angle_beta 69.36
_cell_angle_gamma 90.00
_cell_volume 1821.72
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.00928 0.76418 0.49930
H*2 H -0.02619 0.82445 0.57081
H*3 H -0.01312 0.77167 0.42670
H*4 H 0.06727 0.80378 0.46699
C1+ C 0.72342 0.03775 -0.10144

N'2+ N 0.59344 0.02510 -0.00459
N3+ N 0.61528 0.01130 -0.12994
N'4+ N 0.69403 0.01748 -0.19620
N'5+ N 0.66372 0.04189 0.01485
C6+ C 0.81354 0.04684 -0.12567
N7+ N 0.83046 0.04964 0.00106
O8+ O 0.86762 -0.04375 0.02348
O9+ O 0.80412 0.14809 0.06510
N10+ N 0.85928 -0.07584 -0.20501
O11+ O 0.82363 -0.18086 -0.17149
O12+ O 0.92486 -0.05544 -0.28985
N13+ N 0.85625 0.17303 -0.20175
O14+ O 0.82410 0.21964 -0.27284
O15+ O 0.91838 0.20969 -0.18467
O16+ O 0.55992 -0.00789 -0.18885
H*17+ H 0.50647 -0.00992 -0.11961

#END

data_FTNM_2O_NH3_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 8.180
_cell_length_b 5.976
_cell_length_c 20.904
_cell_angle_alpha 90.00
_cell_angle_beta 117.56
_cell_angle_gamma 90.00
_cell_volume 905.91
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.60186 0.24070 0.61325
H*2 H 0.71704 0.16535 0.65188
H*3 H 0.50745 0.24452 0.63225
H*4 H 0.63633 0.40252 0.60981
C1+ C -0.05512 0.79265 0.10383
N'2+ N -0.33532 0.68780 0.05267
N3+ N -0.22984 0.56752 0.03299
N'4+ N -0.05591 0.62099 0.06216
N'5+ N -0.22215 0.83460 0.09912

C6+ C 0.11755 0.91215 0.15252
N7+ N 0.08379 1.07787 0.20205
O8+ O 0.16086 1.04023 0.26636
O9+ O -0.01835 1.23143 0.16993
N10+ N 0.26788 0.74053 0.20119
O11+ O 0.21070 0.59181 0.22506
O12+ O 0.42413 0.77216 0.21091
N13+ N 0.20399 1.05195 0.11264
O14+ O 0.17108 0.98572 0.05298
O15+ O 0.29912 1.20901 0.14601
O16+ O -0.29573 0.39727 -0.01504
H*17+ H -0.42645 0.38992 -0.02807

#END

data_FTNM_2O_NH3_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 16.339
_cell_length_b 10.487
_cell_length_c 11.144
_cell_angle_alpha 90.00
_cell_angle_beta 105.34
_cell_angle_gamma 90.00
_cell_volume 1841.46
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.91964 0.79511 0.09834
H*2 H 0.97608 0.76647 0.08465
H*3 H 0.87670 0.79582 0.01331
H*4 H 0.90093 0.72580 0.14946
C1+ C 0.72503 0.55861 0.35988
N'2+ N 0.59082 0.56339 0.32737
N3+ N 0.61526 0.54629 0.22411
N'4+ N 0.69669 0.54190 0.23625
N'5+ N 0.66211 0.57103 0.41650

C6+ C 0.81702 0.55602 0.42512
N7+ N 0.83105 0.55788 0.56794
O8+ O 0.86301 0.46430 0.62562
O9+ O 0.80810 0.65582 0.60703
N10+ N 0.85863 0.43240 0.38965
O11+ O 0.81626 0.33672 0.38613
O12+ O 0.92800 0.44302 0.37050
N13+ N 0.86870 0.67064 0.39361
O14+ O 0.84054 0.71842 0.29179
O15+ O 0.93289 0.69824 0.47264
O16+ O 0.55989 0.53415 0.11045
H*17+ H 0.50413 0.53943 0.12637

#END

data_FTNM_2O_NH3_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 8.529
_cell_length_b 11.718
_cell_length_c 11.405
_cell_angle_alpha 90.00
_cell_angle_beta 52.09
_cell_angle_gamma 90.00
_cell_volume 899.314
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.17492 -0.71267 0.33908
H*2 H -0.22974 -0.63163 0.36630
H*3 H -0.23385 -0.75121 0.29400
H*4 H -0.02576 -0.70618 0.25662
C1+ C 0.24180 0.26758 0.33702
N'2+ N 0.06987 0.12576 0.47292
N3+ N 0.15671 0.10829 0.33020
N'4+ N 0.26537 0.19119 0.23943
N'5+ N 0.12531 0.22940 0.47825
C6+ C 0.34528 0.37968 0.28862
N7+ N 0.31639 0.44287 0.41976
O8+ O 0.46274 0.45871 0.41245
O9+ O 0.14576 0.47052 0.51746

N10+ N 0.57286 0.36199 0.16386
O11+ O 0.64375 0.28278 0.18564
O12+ O 0.65586 0.42800 0.06010
N13+ N 0.27277 0.46331 0.22432
O14+ O 0.20526 0.41889 0.16781
O15+ O 0.29593 0.56405 0.23384
O16+ O 0.13574 0.01030 0.27817
H*17+ H 0.05074 -0.03736 0.36613

#END

data_FTNM_2O_NH3_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 15.342
_cell_length_b 10.371
_cell_length_c 11.917
_cell_angle_alpha 90.00
_cell_angle_beta 70.35
_cell_angle_gamma 90.00
_cell_volume 1785.71
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.39319 0.44072 0.19987
H*2 H 0.36176 0.49106 0.27626
H*3 H 0.46056 0.46977 0.16881
H*4 H 0.39317 0.34625 0.22339
C1+ C -0.01170 0.27291 0.47829
N'2+ N -0.15793 0.27696 0.52180
N3+ N -0.11561 0.21004 0.42373
N'4+ N -0.02580 0.20265 0.39121
N'5+ N -0.09060 0.31792 0.55823
C6+ C 0.08220 0.29101 0.48621
N7+ N 0.07688 0.35844 0.60413
O8+ O 0.10140 0.29713 0.67493
O9+ O 0.04828 0.46832 0.61225

N10+ N 0.13048 0.15744 0.48124
O11+ O 0.08026 0.07371 0.53982
O12+ O 0.21181 0.15028 0.42169
N13+ N 0.14870 0.37438 0.38391
O14+ O 0.13357 0.37289 0.29025
O15+ O 0.21015 0.42948 0.40734
O16+ O -0.16152 0.15164 0.35860
H*17+ H -0.22654 0.17019 0.40141

#END

S56. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 5-(trinitromethyl)tetrazole 2*N*-oxide (cocrystal form).
data_FTNM_2O_NH2OH_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 8.198
_cell_length_b 10.452
_cell_length_c 5.831
_cell_angle_alpha 77.12
_cell_angle_beta 110.98
_cell_angle_gamma 96.39
_cell_volume 454.499
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.29217 0.49138 0.06747
H*2 H -0.22207 0.41215 0.08738
H*3 H -0.36894 0.46003 0.17535
O4 O -0.41442 0.50624 -0.18644
H*5 H -0.39220 0.59611 -0.25802
C1+ C 0.09269 0.24578 0.85286
N'2+ N -0.08769 0.33342 0.95280
N3+ N -0.14096 0.33225 0.71000
N'4+ N -0.03776 0.27978 0.63378
N'5+ N 0.06445 0.27668 1.04758
C6+ C 0.24615 0.17478 0.87296
N7+ N 0.36186 0.13027 1.15013
O8+ O 0.37282 0.01311 1.23336
O9+ O 0.43093 0.22032 1.25518
N10+ N 0.18367 0.05036 0.75323
O11+ O 0.06185 -0.01090 0.80290
O12+ O 0.26172 0.02646 0.62682

N13+ N 0.36882 0.25726 0.73861
O14+ O 0.29956 0.34310 0.56153
O15+ O 0.51978 0.22507 0.82052
O16+ O -0.29392 0.38270 0.54498
H*17+ H -0.34642 0.41416 0.64709

#END

data_FTNM_2O_NH2OH_2
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 8.390
_cell_length_b 11.593
_cell_length_c 5.795
_cell_angle_alpha 79.16
_cell_angle_beta 77.28
_cell_angle_gamma 57.48
_cell_volume 461.942
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.18577 0.51123 -0.06455
H*2 H -0.09853 0.54481 -0.16124
H*3 H -0.32163 0.59417 -0.06388
O4 O -0.14989 0.49262 0.17647
H*5 H -0.11438 0.39833 0.22339
C1+ C -0.12518 0.24234 0.76888
N'2+ N -0.42123 0.32712 0.89644
N3+ N -0.38285 0.32973 0.66158
N'4+ N -0.20424 0.27920 0.56942
N'5+ N -0.25367 0.26973 0.96791
C6+ C 0.08483 0.17172 0.76374
N7+ N 0.13868 0.12244 1.01759
O8+ O 0.23286 -0.00040 1.06724
O9+ O 0.07938 0.21510 1.14116
N10+ N 0.18930 0.04391 0.61652
O11+ O 0.11308 -0.02325 0.65338
O12+ O 0.33414 0.02346 0.48399
N13+ N 0.17216 0.26262 0.64994
O14+ O 0.08641 0.35368 0.50279
O15+ O 0.31940 0.23091 0.71542
O16+ O -0.51941 0.38204 0.52002
H*17+ H -0.63806 0.41138 0.62989

```
#END

data_FTNM_2O_NH2OH_3
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 8.435
_cell_length_b                 12.644
_cell_length_c                 5.809
_cell_angle_alpha               111.31
_cell_angle_beta                75.56
_cell_angle_gamma                 65.74
_cell_volume                   464.639
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.68731 0.48932 0.04529
H*2 H 0.82910 0.40621 -0.05901
H*3 H 0.60089 0.45709 0.10672
O4 O 0.65163 0.50715 -0.17289
H*5 H 0.61048 0.60058 -0.10750
C1+ C 0.39699 0.24250 0.44203
N'2+ N 0.09514 0.31960 0.66859
N3+ N 0.13497 0.32773 0.44222
N'4+ N 0.31717 0.28215 0.29138
N'5+ N 0.26559 0.26357 0.66938
C6+ C 0.61152 0.17555 0.35156
N7+ N 0.66770 0.12186 0.53853
O8+ O 0.77526 -0.00075 0.42936
O9+ O 0.59622 0.21125 0.77974
N10+ N 0.73201 0.05217 0.04247
O11+ O 0.66591 -0.01738 -0.01209
O12+ O 0.87773 0.03700 -0.10976
N13+ N 0.68624 0.27071 0.36196
O14+ O 0.59219 0.36357 0.33373
O15+ O 0.83352 0.24022 0.38987
O16+ O -0.00371 0.38064 0.36684
H*17+ H -0.12474 0.40569 0.50937

#END

data_FTNM_2O_NH2OH_4
_symmetry_cell_setting          monoclinic
```

```
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 15.745
_cell_length_b                 5.821
_cell_length_c                 20.456
_cell_angle_alpha               90.00
_cell_angle_beta                86.19
_cell_angle_gamma                 90.00
_cell_volume                   1870.68
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.60153 0.04676 0.50392
H*2 H 0.56402 -0.08913 0.51892
H*3 H 0.63431 0.09119 0.54351
O4 O 0.54188 0.23325 0.49809
H*5 H 0.55396 0.28383 0.45351
C1+ C 0.28848 -0.03818 0.12621
N'2+ N 0.19946 0.18078 0.08334
N3+ N 0.17573 -0.03785 0.08435
N'4+ N 0.22684 -0.18311 0.11006
N'5+ N 0.27285 0.18215 0.11081
C6+ C 0.36318 -0.11780 0.16084
N7+ N 0.41691 0.08803 0.18227
O8+ O 0.42060 0.12011 0.24061
O9+ O 0.45045 0.19635 0.13693
N10+ N 0.33277 -0.25743 0.22330
O11+ O 0.27195 -0.17483 0.25445
O12+ O 0.37224 -0.42992 0.23491
N13+ N 0.42543 -0.27724 0.11916
O14+ O 0.39382 -0.38833 0.07680
O15+ O 0.49856 -0.27853 0.13439
O16+ O 0.10260 -0.11165 0.06007
H*17+ H 0.07599 0.02753 0.04458

#END

data_FTNM_2O_NH2OH_5
```

```
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number     2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                  8.556
_cell_length_b                  7.598
_cell_length_c                  7.281
_cell_angle_alpha                87.03
_cell_angle_beta                 88.68
_cell_angle_gamma                   84.68
_cell_volume                    470.576
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.99109 -0.29023 0.46281
H*2 H -1.07050 -0.37049 0.41853
H*3 H -0.95187 -0.22457 0.34716
O4 O -0.85811 -0.41171 0.51692
H*5 H -0.84283 -0.38300 0.64244
C1+ C 0.58789 -0.24773 0.78892
N'2+ N 0.36052 -0.30529 0.71215
N3+ N 0.46062 -0.29912 0.57066
N'4+ N 0.60281 -0.26499 0.60645
N'5+ N 0.44286 -0.27255 0.85529
C6+ C 0.72299 -0.21424 0.90294
N7+ N 0.67928 -0.22743 1.11024
O8+ O 0.74722 -0.34619 1.20358
O9+ O 0.57956 -0.11368 1.15713
N10+ N 0.86493 -0.35352 0.86643
O11+ O 0.82947 -0.50361 0.85568
O12+ O 0.99429 -0.30036 0.85419
N13+ N 0.78416 -0.02822 0.86496
O14+ O 0.76274 0.03792 0.71116
O15+ O 0.85046 0.02935 0.99127
O16+ O 0.42037 -0.32579 0.39619
H*17+ H 0.31051 -0.34999 0.40624

#END
```

S57. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 5-(trinitromethyl)tetrazole 2*N*-oxide (cocrystal form).

```
data_FTNM_2O_N2H4_1
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number     2
```

```
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 9.128
_cell_length_b                 8.001
_cell_length_c                 8.447
_cell_angle_alpha               71.45
_cell_angle_beta                77.86
_cell_angle_gamma                52.00
_cell_volume                   460.79
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.17169 -0.08040 0.82222
H*2 H 0.14532 0.06779 0.80570
H*3 H 0.05251 -0.06583 0.86529
N4 N 0.31225 -0.24814 0.94413
H*5 H 0.43751 -0.31575 0.88307
H*6 H 0.31460 -0.18670 1.03172
C1+ C -0.04650 0.34787 0.34203
N'2+ N -0.29117 0.40494 0.47850
N3+ N -0.31790 0.48960 0.31549
N'4+ N -0.17430 0.46108 0.22297
N'5+ N -0.11413 0.31137 0.49681
C6+ C 0.15085 0.26369 0.30110
N7+ N 0.27256 0.11166 0.45766
O8+ O 0.39104 -0.07951 0.45785
O9+ O 0.23487 0.20406 0.56516
N10+ N 0.22886 0.13073 0.16589
O11+ O 0.18315 0.01103 0.18751
O12+ O 0.32675 0.15729 0.05548
N13+ N 0.18233 0.44521 0.23041
O14+ O 0.05212 0.62167 0.15744
O15+ O 0.33515 0.39010 0.25173
O16+ O -0.48455 0.60149 0.24517
H*17+ H -0.56669 0.59814 0.33879

#END

data_FTNM_2O_N2H4_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 17.445
_cell_length_b 10.217
_cell_length_c 11.323
_cell_angle_alpha 90.00
_cell_angle_beta 70.23
_cell_angle_gamma 90.00
_cell_volume 1899.21
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.02189 0.74539 0.55806
H*2 H 0.08263 0.74304 0.54523
H*3 H -0.00841 0.70737 0.64425
N4 N 0.00206 0.66695 0.46708
H*5 H 0.00706 0.72496 0.39187
H*6 H 0.04129 0.59033 0.43647
C1+ C 0.21843 0.04064 0.40070
N'2+ N 0.09028 0.03112 0.49345
N3+ N 0.11206 0.00722 0.37140
N'4+ N 0.18972 0.01084 0.30782
N'5+ N 0.15940 0.05254 0.51343
C6+ C 0.30718 0.05144 0.37872
N7+ N 0.32351 0.06644 0.50409
O8+ O 0.35985 -0.02146 0.53424
O9+ O 0.29761 0.16763 0.55921
N10+ N 0.35216 -0.07402 0.31086
O11+ O 0.31682 -0.17563 0.35072
O12+ O 0.41694 -0.05873 0.22752
N13+ N 0.34961 0.17027 0.29549
O14+ O 0.31824 0.20809 0.22093
O15+ O 0.41076 0.21060 0.31143
O16+ O 0.05770 -0.01946 0.31307
H*17+ H 0.00494 -0.01760 0.38001

#END

data_FTNM_2O_N2H4_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id

```
_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
_cell_length_a                 15.475
_cell_length_b                 10.890
_cell_length_c                 11.561
_cell_angle_alpha               90.00
_cell_angle_beta                88.37
_cell_angle_gamma                 90.00
_cell_volume                   1947.5
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.74490 0.06294 0.34431
H*2 H 0.79728 0.04544 0.29131
H*3 H 0.74263 -0.00288 0.40670
N4 N 0.66531 0.05693 0.28354
H*5 H 0.65334 0.14216 0.25186
H*6 H 0.66919 -0.00226 0.21520
C1+ C 0.48309 0.27945 -0.01377
N'2+ N 0.34788 0.28239 0.02449
N3+ N 0.36828 0.21840 -0.06999
N'4+ N 0.45004 0.21189 -0.09914
N'5+ N 0.42251 0.32216 0.06197
C6+ C 0.57778 0.29748 -0.00332
N7+ N 0.59844 0.36238 0.11166
O8+ O 0.63867 0.30463 0.18190
O9+ O 0.57151 0.46684 0.11837
N10+ N 0.62499 0.17065 -0.00628
O11+ O 0.58856 0.09087 0.04987
O12+ O 0.69236 0.16412 -0.06213
N13+ N 0.62063 0.37678 -0.10178
O14+ O 0.58485 0.37467 -0.19387
O15+ O 0.68650 0.42990 -0.07724
O16+ O 0.30856 0.16202 -0.13486
H*17+ H 0.25359 0.17942 -0.09495

#END

data_FTNM_2O_N2H4_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
```

```
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 14.947
_cell_length_b                 10.169
_cell_length_c                 8.232
_cell_angle_alpha               90.00
_cell_angle_beta                52.69
_cell_angle_gamma                 90.00
_cell_volume                   995.189
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.47473 0.23417 -0.10954
H*2 H 0.40986 0.24131 -0.11878
H*3 H 0.50746 0.14211 -0.15498
N4 N 0.43787 0.25156 0.09584
H*5 H 0.44214 0.34922 0.11693
H*6 H 0.35655 0.22230 0.20137
C1+ C 0.19400 0.08307 0.60149
N'2+ N 0.06806 0.00884 0.58121
N3+ N 0.13273 0.09907 0.44070
N'4+ N 0.21226 0.14921 0.44256
N'5+ N 0.10779 -0.00255 0.68633
C6+ C 0.26735 0.10014 0.66554
N7+ N 0.23830 -0.00179 0.83056
O8+ O 0.30944 -0.08289 0.78578
O9+ O 0.14512 0.01186 0.99080
N10+ N 0.39339 0.08158 0.47814
O11+ O 0.41027 -0.00922 0.36701
O12+ O 0.46110 0.15697 0.46246
N13+ N 0.25849 0.23810 0.75754
O14+ O 0.23165 0.32811 0.69828
O15+ O 0.28212 0.24204 0.87476
O16+ O 0.11861 0.13938 0.30082
H*17+ H 0.05568 0.08718 0.33002

#END

data_FTNM_2O_N2H4_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
```

```
_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
_cell_length_a                 13.847
_cell_length_b                 12.100
_cell_length_c                 5.792
_cell_angle_alpha               90.00
_cell_angle_beta                103.23
_cell_angle_gamma               90.00
_cell_volume                   944.686
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.19995 0.40107 0.89602
H*2 H 0.23837 0.46662 0.98239
H*3 H 0.14838 0.43111 0.75611
N4 N 0.14815 0.34106 1.04453
H*5 H 0.19489 0.28191 1.13104
H*6 H 0.12879 0.39056 1.16921
C1+ C 0.23985 0.12742 0.63083
N'2+ N 0.09946 0.05375 0.61994
N3+ N 0.11309 0.07790 0.40631
N'4+ N 0.19755 0.12306 0.39781
N'5+ N 0.18205 0.08544 0.76747
C6+ C 0.34249 0.16937 0.72111
N7+ N 0.37789 0.14938 0.99109
O8+ O 0.44652 0.08597 1.05695
O9+ O 0.33182 0.20130 1.10946
N10+ N 0.41539 0.10883 0.59367
O11+ O 0.40104 0.01014 0.56879
O12+ O 0.47853 0.16448 0.53482
N13+ N 0.35511 0.29573 0.68191
O14+ O 0.29713 0.33597 0.51357
O15+ O 0.42312 0.34030 0.81972
O16+ O 0.04396 0.05794 0.20411
H*17+ H -0.01084 0.02362 0.25733

#END
```

S58. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 5-(trinitromethyl)tetrazole 2*N*-oxide (cocrystal form).

```
data_FTNM_2O_G_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
```

```
_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
_cell_length_a                 7.271
_cell_length_b                 14.725
_cell_length_c                 10.206
_cell_angle_alpha               90.00
_cell_angle_beta                106.38
_cell_angle_gamma                 90.00
_cell_volume                   1048.36
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.21085 0.66018 0.62552
N'2 N 0.16814 0.69828 0.72635
H*3 H 0.27784 0.73797 0.78150
N4 N 0.08906 0.59532 0.54651
H*5 H 0.07355 0.59923 0.44480
H*6 H -0.03767 0.59150 0.56925
N7 N 0.37249 0.67632 0.58026
H*8 H 0.47573 0.71358 0.64521
H*9 H 0.42517 0.62109 0.54369
C1+ C 0.88140 -0.03423 0.22755
N'2+ N 0.68466 0.03463 0.31237
N3+ N 0.67465 0.06197 0.18673
N'4+ N 0.79044 0.02280 0.12742
N'5+ N 0.81880 -0.02843 0.33958
C6+ C 1.02821 -0.09969 0.20976
N7+ N 1.08766 -0.16609 0.33192
O8+ O 1.04855 -0.24571 0.30940
O9+ O 1.16966 -0.12987 0.43926
N10+ N 0.94654 -0.15636 0.07657
O11+ O 0.78212 -0.18131 0.05832
O12+ O 1.05288 -0.17051 0.00618
N13+ N 1.21720 -0.05472 0.19760
O14+ O 1.20122 0.02186 0.15167
O15+ O 1.35985 -0.10163 0.23191
O16+ O 0.55220 0.12735 0.12096
H*17+ H 0.48166 0.14473 0.18533

#END

data_FTNM_2O_G_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
```

```
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.434
_cell_length_b                 9.061
_cell_length_c                 10.256
_cell_angle_alpha               90.00
_cell_angle_beta               107.36
_cell_angle_gamma                90.00
_cell_volume                   1102.85
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.75037 -0.15306 0.45039
N'2 N 0.79783 -0.10531 0.36318
H*3 H 0.74171 -0.05122 0.28458
N4 N 0.80936 -0.24406 0.55750
H*5 H 0.79602 -0.22306 0.64852
H*6 H 0.89215 -0.25118 0.56416
N7 N 0.64078 -0.12355 0.45373
H*8 H 0.59088 -0.07464 0.36839
H*9 H 0.60211 -0.20816 0.48644
C1+ C 0.20727 0.81188 0.06022
N'2+ N 0.03652 0.75782 0.03930
N3+ N 0.07488 0.69329 -0.05406
N'4+ N 0.17909 0.72056 -0.04792
N'5+ N 0.12257 0.83499 0.11464
C6+ C 0.32306 0.87259 0.11581
N7+ N 0.33678 0.95515 0.25185
O8+ O 0.40210 0.90378 0.35431
O9+ O 0.27924 1.06537 0.23995
N10+ N 0.41136 0.74480 0.14303
O11+ O 0.38451 0.63571 0.19458
O12+ O 0.49684 0.76639 0.11205
N13+ N 0.35727 0.98445 0.01936
O14+ O 0.31070 0.96830 -0.10192
O15+ O 0.42898 1.07367 0.07500
O16+ O 0.01088 0.60346 -0.15233
H*17+ H -0.06173 0.59999 -0.13426

#END

data_FTNM_2O_G_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
```

```
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 5.701
_cell_length_b                 12.252
_cell_length_c                 14.828
_cell_angle_alpha               90.00
_cell_angle_beta                77.16
_cell_angle_gamma                 90.00
_cell_volume                   1009.82
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74687 0.73966 0.54709
N'2 N 0.65201 0.81679 0.50850
H*3 H 0.77075 0.84720 0.45227
N4 N 0.62377 0.69541 0.63092
H*5 H 0.63789 0.61331 0.63624
H*6 H 0.45169 0.72239 0.64907
N7 N 0.97048 0.68999 0.51417
H*8 H 1.07779 0.72918 0.46042
H*9 H 1.05850 0.66748 0.56357
C1+ C -0.30495 0.53589 0.20909
N'2+ N -0.52797 0.47495 0.12307
N3+ N -0.29937 0.44601 0.09431
N'4+ N -0.15103 0.47993 0.14355
N'5+ N -0.53330 0.53330 0.19819
C6+ C -0.22656 0.58917 0.28756
N7+ N -0.44502 0.63298 0.35978
O8+ O -0.48719 0.59136 0.43591
O9+ O -0.55162 0.70640 0.33124
N10+ N -0.08972 0.50535 0.33649
O11+ O -0.18089 0.41538 0.34680
O12+ O 0.08918 0.53741 0.35980
N13+ N -0.05342 0.68819 0.25927
O14+ O 0.06902 0.68596 0.18103
O15+ O -0.05415 0.75586 0.31901
O16+ O -0.21872 0.38467 0.01775
H*17+ H -0.36215 0.36935 -0.00564

#END

data_FTNM_2O_G_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
```

```
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   6.472
_cell_length_b                   16.764
_cell_length_c                   10.010
_cell_angle_alpha                 90.00
_cell_angle_beta                  93.86
_cell_angle_gamma                    90.00
_cell_volume                     1083.59
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.41953 -0.17234 0.65017
N'2 N -0.50258 -0.15399 0.75906
H*3 H -0.41970 -0.11083 0.81073
N4 N -0.49565 -0.23625 0.57248
H*5 H -0.50150 -0.22697 0.47223
H*6 H -0.63003 -0.25776 0.60449
N7 N -0.25339 -0.13418 0.59442
H*8 H -0.17701 -0.09467 0.65610
H*9 H -0.15687 -0.17064 0.54709
C1+ C 0.11284 0.13876 0.76838
N'2+ N -0.10802 0.22181 0.83283
N3+ N -0.07460 0.22937 0.70417
N'4+ N 0.05849 0.18041 0.65680
N'5+ N 0.01318 0.16257 0.87537
C6+ C 0.26020 0.07073 0.76801
N7+ N 0.27033 0.02607 0.90354
O8+ O 0.20833 -0.04222 0.90335
O9+ O 0.34201 0.06555 0.99710
N10+ N 0.18985 0.01039 0.65497
O11+ O 0.00480 -0.00229 0.64488
O12+ O 0.32350 -0.01803 0.59023
N13+ N 0.48749 0.09487 0.74323
O14+ O 0.50700 0.15528 0.67838
O15+ O 0.62118 0.04977 0.78823
O16+ O -0.17107 0.28476 0.62371
H*17+ H -0.26227 0.31274 0.68160

#END

data_FTNM_2O_G_5
_symmetry_cell_setting           orthorhombic
```

```
_symmetry_space_group_name_H-M   'P c a 21'
_symmetry_Int_Tables_number      29
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                   15.763
_cell_length_b                   6.550
_cell_length_c                   10.232
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
_cell_angle_gamma                    90.00
_cell_volume                     1056.43
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.82276 0.37802 -0.16446
N'2 N -0.82846 0.45176 -0.28046
H*3 H -0.87002 0.37000 -0.33621
N4 N -0.76240 0.45351 -0.07738
H*5 H -0.78270 0.46865 0.01612
H*6 H -0.73340 0.58054 -0.11198
N7 N -0.87245 0.22341 -0.10932
H*8 H -0.90897 0.14683 -0.17416
H*9 H -0.84152 0.12958 -0.04655
C1+ C -0.62048 0.08051 0.75994
N'2+ N -0.70838 -0.14701 0.82032
N3+ N -0.71010 -0.11353 0.69252
N'4+ N -0.65785 0.02355 0.64767
N'5+ N -0.64979 -0.02148 0.86499
C6+ C -0.55073 0.23325 0.76294
N7+ N -0.51076 0.24672 0.90075
O8+ O -0.43748 0.19319 0.91239
O9+ O -0.55862 0.31197 0.98367
N10+ N -0.47977 0.17183 0.66383
O11+ O -0.46293 -0.00899 0.66317
O12+ O -0.44835 0.30737 0.59921
N13+ N -0.57852 0.45481 0.72633
O14+ O -0.63937 0.46804 0.65408
O15+ O -0.53524 0.59105 0.77098
O16+ O -0.76300 -0.21385 0.61040
H*17+ H -0.79426 -0.30743 0.66668

#END
```

S59. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 5-(trinitromethyl)tetrazole 2*N*-oxide (cocrystal form).

```
data_FTNM_2O_AG_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 16.280
_cell_length_b                 6.488
_cell_length_c                 11.084
_cell_angle_alpha               90.00
_cell_angle_beta               105.76
_cell_angle_gamma                90.00
_cell_volume                   1126.73
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.40994 0.78108 0.49133
N2 N 0.44101 0.83356 0.61758
H*3 H 0.41319 0.96077 0.64237
N'4 N 0.46319 0.73022 0.42851
N5 N 0.32203 0.78987 0.44462
H*6 H 0.28953 0.75399 0.50784
H*7 H 0.30219 0.71200 0.36209
N8 N 0.41932 0.65903 0.30372
H*9 H 0.41690 0.78089 0.24432
H*10 H 0.45999 0.55669 0.28060
H*11 H 0.50562 0.84370 0.64362
C1+ C 0.25859 0.67134 -0.21786
N'2+ N 0.12497 0.67036 -0.30479
N3+ N 0.16968 0.75012 -0.37719
N'4+ N 0.25220 0.75574 -0.33075
N'5+ N 0.18257 0.61781 -0.20078
C6+ C 0.34263 0.63296 -0.12623
N7+ N 0.33206 0.50650 -0.01307
O8+ O 0.36263 0.33476 0.00121
O9+ O 0.29357 0.59664 0.05054
N10+ N 0.40188 0.50983 -0.19013
O11+ O 0.36636 0.37131 -0.25812
O12+ O 0.47616 0.56158 -0.16562
N13+ N 0.39236 0.83242 -0.07072
O14+ O 0.37713 0.98413 -0.13721
O15+ O 0.44277 0.81438 0.03174
```

```
O16+ O 0.13319 0.82385 -0.49371
H*17+ H 0.07227 0.80053 -0.50655

#END

data_FTNM_2O_AG_2
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 8.506
_cell_length_b                 6.437
_cell_length_c                 10.992
_cell_angle_alpha               97.35
_cell_angle_beta                94.90
_cell_angle_gamma               105.55
_cell_volume                   570.521
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.67733 0.21267 0.67766
N2 N 0.60415 0.30297 0.58741
H*3 H 0.66428 0.31764 0.51173
N'4 N 0.69359 0.30001 0.79240
N5 N 0.72725 0.03258 0.63323
H*6 H 0.65571 -0.06198 0.55701
H*7 H 0.74820 -0.05133 0.70245
N8 N 0.75495 0.17115 0.87364
H*9 H 0.87888 0.24189 0.89466
H*10 H 0.70787 0.19864 0.95433
H*11 H 0.58448 0.44568 0.62339
C1+ C 0.71430 0.23555 0.22783
N'2+ N 0.52978 0.37821 0.28681
N3+ N 0.52101 0.33563 0.16475
N'4+ N 0.62972 0.24733 0.12119
N'5+ N 0.65527 0.31257 0.32870
C6+ C 0.85277 0.13533 0.23047
N7+ N 0.91105 0.11277 0.36410
O8+ O 0.89209 -0.07045 0.38810
O9+ O 0.97138 0.28609 0.43137
N10+ N 0.79725 -0.09703 0.15087
O11+ O 0.66070 -0.20516 0.16372
O12+ O 0.89386 -0.14728 0.08610
N13+ N 1.00810 0.26688 0.17871
O14+ O 0.98268 0.37800 0.10207
```

O15+ O 1.13784 0.24041 0.21787
O16+ O 0.40660 0.38047 0.08697
H*17+ H 0.34047 0.44254 0.14135

#END

data_FTNM_2O_AG_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 6.560
_cell_length_b 16.569
_cell_length_c 10.777
_cell_angle_alpha 90.00
_cell_angle_beta 91.23
_cell_angle_gamma 90.00
_cell_volume 1171.11
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.40150 0.81217 0.11385
N2 N -0.50834 0.75897 0.03608
H*3 H -0.54200 0.78199 -0.04916
N'4 N -0.45521 0.81966 0.22806
N5 N -0.24358 0.85313 0.05844
H*6 H -0.17263 0.82148 -0.00851
H*7 H -0.14735 0.87779 0.12335
N8 N -0.31413 0.87035 0.29799
H*9 H -0.37722 0.92675 0.30086
H*10 H -0.31913 0.84979 0.38691
H*11 H -0.63357 0.73658 0.07766
C1+ C 0.09096 0.12132 0.27299
N'2+ N -0.13944 0.19746 0.34463
N3+ N -0.10380 0.21134 0.22586
N'4+ N 0.03515 0.16692 0.17491
N'5+ N -0.01345 0.13856 0.37598
C6+ C 0.24512 0.05597 0.26331
N7+ N 0.25712 0.00535 0.38386
O8+ O 0.20524 -0.06481 0.37722
O9+ O 0.31966 0.04268 0.47373
N10+ N 0.18726 -0.00151 0.15316
O11+ O 0.00710 -0.01787 0.14501

O12+ O 0.32450 -0.02447 0.08832
N13+ N 0.46634 0.08630 0.23982
O14+ O 0.47935 0.15040 0.18600
O15+ O 0.60266 0.04181 0.27480
O16+ O -0.20382 0.26853 0.15864
H*17+ H -0.29902 0.29227 0.21649

#END

data_FTNM_2O_AG_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 6.925
_cell_length_b 15.160
_cell_length_c 11.655
_cell_angle_alpha 90.00
_cell_angle_beta 70.06
_cell_angle_gamma 90.00
_cell_volume 1150.22
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.22016 0.83638 0.35648
N2 N -0.26687 0.81039 0.25415
H*3 H -0.36364 0.75803 0.26938
N'4 N -0.03185 0.85457 0.34471
N5 N -0.38648 0.83986 0.46409
H*6 H -0.52069 0.85708 0.45338
H*7 H -0.35227 0.87540 0.52873
N8 N -0.01586 0.88952 0.45685
H*9 H 0.02661 0.83828 0.50018
H*10 H 0.10847 0.93025 0.43012
H*11 H -0.13788 0.80083 0.18078
C1+ C 0.12600 0.45325 0.21529
N'2+ N -0.15444 0.51670 0.31616
N3+ N -0.07878 0.54398 0.20132
N'4+ N 0.09280 0.50801 0.13327
N'5+ N -0.02206 0.45721 0.32590
C6+ C 0.30415 0.39192 0.18196
N7+ N 0.28786 0.32745 0.28775
O8+ O 0.26610 0.24974 0.27051

```
O9+ O 0.29988 0.36304 0.37830
N10+ N 0.31207 0.33665 0.06729
O11+ O 0.14601 0.31020 0.06838
O12+ O 0.47939 0.32491 -0.00973
N13+ N 0.51726 0.43836 0.15021
O14+ O 0.52694 0.51280 0.11020
O15+ O 0.65292 0.39461 0.16570
O16+ O -0.17131 0.60617 0.15465
H*17+ H -0.29529 0.62158 0.22217

#END

data_FTNM_2O_AG_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 15.439
_cell_length_b                 7.069
_cell_length_c                 12.494
_cell_angle_alpha               90.00
_cell_angle_beta                122.56
_cell_angle_gamma               90.00
_cell_volume                   1149.26
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.61499 0.17892 0.68077
N2 N 0.56014 0.32139 0.59230
H*3 H 0.59046 0.35943 0.54081
N'4 N 0.63367 0.19486 0.79448
N5 N 0.64510 0.03000 0.63600
H*6 H 0.59570 0.00041 0.54274
H*7 H 0.66563 -0.08448 0.69420
N8 N 0.68107 0.02526 0.86852
H*9 H 0.75847 0.04997 0.92293
H*10 H 0.65855 0.01930 0.93152
H*11 H 0.54866 0.43459 0.63313
C1+ C 0.05055 0.33993 0.23630
N'2+ N -0.01960 0.13085 0.28782
N3+ N -0.04847 0.11964 0.16702
N'4+ N -0.00859 0.24272 0.12807
N'5+ N 0.04536 0.27387 0.33385
```

C6+ C 0.11821 0.49715 0.24548
N7+ N 0.18902 0.56425 0.38450
O8+ O 0.28075 0.54030 0.43474
O9+ O 0.14334 0.63591 0.42842
N10+ N 0.18725 0.43017 0.19635
O11+ O 0.22271 0.27252 0.23085
O12+ O 0.19946 0.53978 0.13090
N13+ N 0.05949 0.67639 0.16650
O14+ O -0.02559 0.64834 0.07333
O15+ O 0.10579 0.82477 0.20428
O16+ O -0.11609 -0.01114 0.08588
H*17+ H -0.13341 -0.08576 0.13745

#END

S60. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 5-(trinitromethyl)tetrazole 2*N*-oxide (cocrystal form).

data_FTNM_2O_DAG_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 9.184
_cell_length_b 5.816
_cell_length_c 14.974
_cell_angle_alpha 49.90
_cell_angle_beta 81.23
_cell_angle_gamma 83.28
_cell_volume 604.462
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.18284 0.00608 -0.04333
N'2 N 0.19515 0.28162 -0.13911
N3 N 0.24157 -0.08689 0.05649
H*4 H 0.29078 -0.29384 0.10090
N5 N 0.11673 -0.22050 -0.02865
N6 N 0.32995 0.11476 0.04631
N7 N 0.11870 0.33926 -0.22934
H*8 H 0.18929 0.28446 -0.27333
H*9 H 0.38105 0.25226 -0.03741
H*10 H 0.25999 0.25169 0.05410
H*11 H 0.10487 0.56660 -0.28811
H*12 H 0.06913 -0.37867 0.05381
H*13 H 0.04807 -0.13324 -0.09170

C1+ C -0.37193 -0.02034 0.71033
N'2+ N -0.50878 -0.39736 0.83411
N3+ N -0.58212 -0.15467 0.75146
N'4+ N -0.50589 0.08602 0.67197
N'5+ N -0.37135 -0.31186 0.80762
C6+ C -0.23890 0.16726 0.64576
N7+ N -0.09729 -0.02326 0.69872
O8+ O -0.00992 -0.05494 0.63769
O9+ O -0.08941 -0.12096 0.79796
N10+ N -0.22612 0.30839 0.51410
O11+ O -0.25359 0.13742 0.49886
O12+ O -0.18957 0.56830 0.44124
N13+ N -0.23794 0.43420 0.64657
O14+ O -0.35815 0.53204 0.65625
O15+ O -0.11736 0.52191 0.63441
O16+ O -0.72890 -0.15013 0.74781
H*17+ H -0.75916 -0.35414 0.81481

#END

data_FTNM_2O_DAG_2
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 14.233
_cell_length_b 8.888
_cell_length_c 6.297
_cell_angle_alpha 104.14
_cell_angle_beta 88.22
_cell_angle_gamma 50.95
_cell_volume 581.508
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.79903 -0.29920 -0.25249
N'2 N 0.73528 -0.31957 -0.13128
N3 N 0.74743 -0.19140 -0.40289
H*4 H 0.80968 -0.25887 -0.55183
N5 N 0.92015 -0.38010 -0.25276
N6 N 0.63158 -0.12839 -0.44007
N7 N 0.80046 -0.42202 0.02455
H*8 H 0.85722 -0.57740 -0.05798
H*9 H 0.62427 -0.23105 -0.41695
H*10 H 0.56336 0.00747 -0.31399

H*11 H 0.73380 -0.38733 0.14398
H*12 H 0.93913 -0.29462 -0.28627
H*13 H 0.94312 -0.41464 -0.11000
C1+ C 0.67144 0.18904 0.34690
N'2+ N 0.49244 0.27688 0.39079
N3+ N 0.54739 0.21214 0.17601
N'4+ N 0.65771 0.15489 0.13487
N'5+ N 0.57302 0.26151 0.50339
C6+ C 0.78786 0.13912 0.39594
N7+ N 0.78613 0.16357 0.64821
O8+ O 0.86259 0.00940 0.69310
O9+ O 0.70646 0.33947 0.77584
N10+ N 0.90359 -0.08815 0.25072
O11+ O 0.88901 -0.21033 0.23878
O12+ O 0.99534 -0.12088 0.16718
N13+ N 0.81154 0.27722 0.34398
O14+ O 0.76657 0.34809 0.19719
O15+ O 0.87513 0.29540 0.45126
O16+ O 0.49371 0.20485 0.00455
H*17+ H 0.41378 0.25282 0.07811

#END

data_FTNM_2O_DAG_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 12.264
_cell_length_b 6.018
_cell_length_c 16.416
_cell_angle_alpha 90.00
_cell_angle_beta 91.70
_cell_angle_gamma 90.00
_cell_volume 1211.05
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.73975 -0.05023 0.59374
N'2 N 0.70893 -0.22742 0.63110
N3 N 0.66786 0.12842 0.58322
H*4 H 0.67214 0.20000 0.52749
N5 N 0.84089 -0.01793 0.55985

N6 N 0.55760 0.10058 0.60490
N7 N 0.79655 -0.38596 0.64110
H*8 H 0.79739 -0.48212 0.58970
H*9 H 0.53713 -0.06322 0.59743
H*10 H 0.55435 0.12983 0.66590
H*11 H 0.77314 -0.48984 0.68622
H*12 H 0.86631 0.14240 0.56035
H*13 H 0.89723 -0.12513 0.58410
C1+ C -0.28725 0.44972 0.36036
N'2+ N -0.43506 0.30043 0.39709
N3+ N -0.44685 0.41553 0.32850
N'4+ N -0.35981 0.51174 0.30177
N'5+ N -0.33099 0.32120 0.41811
C6+ C -0.16989 0.51004 0.35721
N7+ N -0.10240 0.38945 0.42493
O8+ O -0.03536 0.25466 0.40380
O9+ O -0.12465 0.44588 0.49341
N10+ N -0.12389 0.44267 0.27298
O11+ O -0.15427 0.26216 0.24838
O12+ O -0.06285 0.57281 0.24112
N13+ N -0.14599 0.76326 0.36824
O14+ O -0.21930 0.88778 0.34691
O15+ O -0.05568 0.81019 0.39500
O16+ O -0.54350 0.43567 0.28714
H*17+ H -0.59432 0.34855 0.31864

#END

data_FTNM_2O_DAG_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 16.868
_cell_length_b 6.653
_cell_length_c 11.131
_cell_angle_alpha 90.00
_cell_angle_beta 100.08
_cell_angle_gamma 90.00
_cell_volume 1229.87
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

C1 C 0.61295 0.12651 0.20596
N'2 N 0.59622 0.31584 0.20850
N3 N 0.63012 0.01722 0.31467
H*4 H 0.67589 -0.08190 0.31557
N5 N 0.61745 0.01502 0.10196
N6 N 0.63871 0.12235 0.42706
N7 N 0.57459 0.39868 0.08741
H*8 H 0.62654 0.44192 0.05900
H*9 H 0.65957 0.26389 0.41432
H*10 H 0.58231 0.14188 0.44613
H*11 H 0.54493 0.52875 0.09818
H*12 H 0.60195 -0.13145 0.10775
H*13 H 0.58761 0.08470 0.02590
C1+ C 0.09366 0.40183 0.74247
N'2+ N 0.01047 0.21110 0.81037
N3+ N 0.01512 0.17409 0.69473
N'4+ N 0.06504 0.28441 0.64642
N'5+ N 0.06179 0.35908 0.84236
C6+ C 0.15737 0.55448 0.73744
N7+ N 0.18770 0.64569 0.86505
O8+ O 0.25706 0.61318 0.91153
O9+ O 0.13721 0.74277 0.90494
N10+ N 0.23049 0.45574 0.69110
O11+ O 0.24887 0.29107 0.73407
O12+ O 0.26177 0.55113 0.61915
N13+ N 0.13006 0.73539 0.65067
O14+ O 0.07618 0.70046 0.56566
O15+ O 0.16678 0.89101 0.67509
O16+ O -0.02919 0.03037 0.62780
H*17+ H -0.06044 -0.03073 0.68402

#END

data_FTNM_2O_DAG_5
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C c'
_symmetry_Int_Tables_number 9
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 11.318
_cell_length_b 11.483
_cell_length_c 10.311
_cell_angle_alpha 90.00
_cell_angle_beta 65.55
_cell_angle_gamma 90.00
_cell_volume 1219.89
loop_

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.58375 0.58605 -0.17940
N'2 N 0.62466 0.69037 -0.22124
N3 N 0.65360 0.49001 -0.25663
H*4 H 0.59562 0.42568 -0.26469
N5 N 0.47100 0.55755 -0.06167
N6 N 0.75970 0.50934 -0.38981
N7 N 0.54513 0.77720 -0.12256
H*8 H 0.46964 0.79635 -0.14917
H*9 H 0.74202 0.58370 -0.43363
H*10 H 0.83824 0.52765 -0.36906
H*11 H 0.60049 0.85051 -0.14538
H*12 H 0.47616 0.48140 -0.01450
H*13 H 0.43999 0.62547 0.00774
C1+ C 0.58589 0.17288 -0.22935
N'2+ N 0.42475 0.10661 -0.26179
N3+ N 0.43823 0.22098 -0.27974
N'4+ N 0.53510 0.26830 -0.26212
N'5+ N 0.52108 0.07447 -0.22941
C6+ C 0.70589 0.17806 -0.20400
N7+ N 0.75365 0.05435 -0.19033
O8+ O 0.85717 0.02333 -0.28147
O9+ O 0.68013 0.00118 -0.08663
N10+ N 0.81611 0.24129 -0.33073
O11+ O 0.82313 0.21403 -0.44744
O12+ O 0.88348 0.30923 -0.30155
N13+ N 0.69024 0.24485 -0.06591
O14+ O 0.60732 0.31996 -0.02653
O15+ O 0.76468 0.21706 -0.01404
O16+ O 0.35671 0.28757 -0.31418
H*17+ H 0.29467 0.23245 -0.32240

#END
```

S61. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 5-(trinitromethyl)tetrazole 2*N*-oxide (cocrystal form).

```
data_FTNM_2O_TAG_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C c'
_symmetry_Int_Tables_number      9
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                  7.161
```

```
_cell_length_b                14.318
_cell_length_c                12.554
_cell_angle_alpha               90.00
_cell_angle_beta                87.13
_cell_angle_gamma                 90.00
_cell_volume                  1285.56
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.21018 0.33487 0.59837
N'2 N 0.34913 0.30091 0.64834
N3 N 0.40802 0.36378 0.73011
N4 N 0.12138 0.41839 0.62730
N5 N 0.00314 0.45847 0.55247
N6 N 0.14183 0.28727 0.51291
N7 N 0.19056 0.19255 0.49662
H*8 H 0.53466 0.33939 0.75054
H*9 H 0.32091 0.35503 0.79659
H*10 H 0.21186 0.46182 0.66337
H*11 H -0.10062 0.49370 0.59331
H*12 H 0.07492 0.50365 0.50275
H*13 H 0.00948 0.30327 0.49513
H*14 H 0.32280 0.19149 0.46256
H*15 H 0.20175 0.16173 0.56964
C1+ C -0.08327 0.85850 0.29079
N'2+ N -0.25129 0.75106 0.22845
N3+ N -0.29474 0.83527 0.19334
N'4+ N -0.19761 0.90495 0.22768
N'5+ N -0.11286 0.76557 0.29180
C6+ C 0.06607 0.90673 0.34786
N7+ N 0.19438 0.83542 0.40100
O8+ O 0.35626 0.83151 0.36791
O9+ O 0.11620 0.79053 0.47203
N10+ N 0.18893 0.96710 0.26788
O11+ O 0.22697 0.92926 0.18304
O12+ O 0.23514 1.04391 0.29757
N13+ N -0.00747 0.97408 0.43835
O14+ O -0.16082 1.00773 0.42703
O15+ O 0.09793 0.98786 0.50936
O16+ O -0.43275 0.85029 0.12548
H*17+ H -0.48166 0.78822 0.11136

#END

data_FTNM_2O_TAG_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
```

```
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 12.160
_cell_length_b                 6.106
_cell_length_c                 20.053
_cell_angle_alpha               90.00
_cell_angle_beta                57.29
_cell_angle_gamma                  90.00
_cell_volume                   1252.8
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.40576 0.10204 0.60234
N'2 N 0.33181 -0.05698 0.64698
N3 N 0.40483 -0.21582 0.66124
N4 N 0.53681 0.12250 0.57734
N5 N 0.61374 0.27109 0.51463
N6 N 0.35499 0.26313 0.57814
N7 N 0.21805 0.28528 0.61701
H*8 H 0.34551 -0.34899 0.68381
H*9 H 0.41383 -0.15894 0.70613
H*10 H 0.57592 -0.02773 0.57443
H*11 H 0.68416 0.33269 0.52192
H*12 H 0.65695 0.19524 0.46088
H*13 H 0.40448 0.40640 0.56157
H*14 H 0.18709 0.16547 0.59547
H*15 H 0.17658 0.24694 0.67560
C1+ C 0.07737 0.27799 0.36724
N'2+ N -0.09931 0.12064 0.39645
N3+ N -0.03582 0.20801 0.32450
N'4+ N 0.07376 0.30706 0.30203
N'5+ N -0.02579 0.16487 0.42464
C6+ C 0.18930 0.35488 0.37164
N7+ N 0.17788 0.27097 0.44794
O8+ O 0.26054 0.14354 0.44022
O9+ O 0.08512 0.34514 0.50850
N10+ N 0.32057 0.26869 0.29869
O11+ O 0.31683 0.07964 0.28132
O12+ O 0.41207 0.39484 0.26741
N13+ N 0.20235 0.60919 0.37200
O14+ O 0.15904 0.71143 0.33920
O15+ O 0.25740 0.67858 0.40317
O16+ O -0.08040 0.19807 0.27561
H*17+ H -0.16166 0.11538 0.30538
```

```
#END

data_FTNM_2O_TAG_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a                 6.425
_cell_length_b                 15.163
_cell_length_c                 13.096
_cell_angle_alpha               90.00
_cell_angle_beta                97.25
_cell_angle_gamma               90.00
_cell_volume                   1265.64
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.56404 -0.28856 0.01718
N'2 N 0.38753 -0.33110 0.00887
N3 N 0.24903 -0.29659 0.07788
N4 N 0.60447 -0.21441 0.07945
N5 N 0.81639 -0.18695 0.10054
N6 N 0.72192 -0.31552 -0.03820
N7 N 0.67454 -0.37437 -0.12153
H*8 H 0.13501 -0.34294 0.07908
H*9 H 0.17484 -0.24208 0.04447
H*10 H 0.51818 -0.21658 0.13968
H*11 H 0.81846 -0.12046 0.10997
H*12 H 0.88891 -0.21588 0.16584
H*13 H 0.82988 -0.26915 -0.04929
H*14 H 0.66409 -0.43581 -0.09097
H*15 H 0.52626 -0.36069 -0.15637
C1+ C 0.07103 -0.03908 0.75252
N'2+ N -0.16607 0.05589 0.70687
N3+ N -0.12447 0.00466 0.62991
N'4+ N 0.01887 -0.05550 0.65171
N'5+ N -0.03966 0.02754 0.78729
C6+ C 0.22775 -0.09360 0.81778
N7+ N 0.23381 -0.06914 0.93280
O8+ O 0.17820 -0.12491 0.98999
O9+ O 0.29613 0.00509 0.95324
N10+ N 0.17028 -0.19345 0.80481
O11+ O -0.01539 -0.20922 0.80286
```

O12+ O 0.31314 -0.24472 0.79897
N13+ N 0.45736 -0.08391 0.79196
O14+ O 0.47501 -0.06383 0.70372
O15+ O 0.59478 -0.09963 0.86187
O16+ O -0.22288 0.01306 0.53272
H*17+ H -0.32218 0.06115 0.53682

#END

data_FTNM_2O_TAG_4
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C c'
_symmetry_Int_Tables_number 9
loop_
_symmetry_equiv_pos_site_id
_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
_cell_length_a 12.963
_cell_length_b 19.246
_cell_length_c 6.204
_cell_angle_alpha 90.00
_cell_angle_beta 120.31
_cell_angle_gamma 90.00
_cell_volume 1336.24
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.16183 0.87412 0.39399
N'2 N 0.18969 0.93029 0.31927
N3 N 0.09246 0.95388 0.08238
N4 N 0.04827 0.84444 0.26792
N5 N 0.03710 0.77549 0.33374
N6 N 0.24609 0.84129 0.60969
N7 N 0.35126 0.87721 0.77925
H*8 H 0.12944 0.98949 0.02035
H*9 H 0.03374 0.98118 0.11464
H*10 H 0.00691 0.85621 0.08238
H*11 H -0.04616 0.76974 0.30857
H*12 H 0.04894 0.74018 0.22552
H*13 H 0.21323 0.80977 0.69112
H*14 H 0.40680 0.87599 0.70762
H*15 H 0.33040 0.92863 0.77705
C1+ C 0.61735 0.12501 -0.06127
N'2+ N 0.46668 0.13480 -0.01354
N3+ N 0.47228 0.07342 -0.10427
N'4+ N 0.56236 0.06324 -0.13831

```
N'5+ N 0.56133 0.16869 0.01597
C6+ C 0.73197 0.14023 -0.05200
N7+ N 0.78446 0.21047 0.07910
O8+ O 0.87844 0.20906 0.27551
O9+ O 0.72404 0.26038 -0.03347
N10+ N 0.82515 0.08191 0.09567
O11+ O 0.82622 0.06279 0.28321
O12+ O 0.88695 0.06208 0.01254
N13+ N 0.72194 0.14487 -0.31318
O14+ O 0.64199 0.11113 -0.47836
O15+ O 0.79685 0.18022 -0.32317
O16+ O 0.38968 0.02295 -0.16124
H*17+ H 0.33349 0.04280 -0.11746

#END

data_FTNM_2O_TAG_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2'
_symmetry_Int_Tables_number      5
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,-z
3 1/2+x,1/2+y,z
4 1/2-x,1/2+y,-z
_cell_length_a                 26.735
_cell_length_b                 6.870
_cell_length_c                 7.752
_cell_angle_alpha               90.00
_cell_angle_beta               111.11
_cell_angle_gamma                90.00
_cell_volume                   1328.25
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.37905 0.63553 -0.31372
N'2 N 0.41993 0.75076 -0.27961
N3 N 0.40368 0.94448 -0.34970
N4 N 0.32613 0.69842 -0.39476
N5 N 0.28629 0.55301 -0.46379
N6 N 0.38685 0.44087 -0.26719
N7 N 0.43732 0.37776 -0.14359
H*8 H 0.43793 1.01147 -0.34627
H*9 H 0.39170 1.01780 -0.25615
H*10 H 0.32403 0.81674 -0.47663
H*11 H 0.25182 0.60260 -0.45245
H*12 H 0.27953 0.52268 -0.59913
```

H*13 H 0.35522 0.37139 -0.25297
H*14 H 0.46211 0.36950 -0.21711
H*15 H 0.45327 0.48580 -0.04857
C1+ C 0.10629 0.54719 -0.15662
N'2+ N 0.02206 0.50546 -0.24062
N3+ N 0.04981 0.34523 -0.17254
N'4+ N 0.10179 0.35896 -0.11739
N'5+ N 0.05865 0.63820 -0.23005
C6+ C 0.15935 0.64290 -0.11193
N7+ N 0.15294 0.86505 -0.14519
O8+ O 0.17078 0.97050 -0.01143
O9+ O 0.13033 0.90956 -0.30611
N10+ N 0.19464 0.60748 0.09546
O11+ O 0.17068 0.62311 0.20126
O12+ O 0.24163 0.57032 0.13080
N13+ N 0.19254 0.56820 -0.22815
O14+ O 0.18355 0.40197 -0.28393
O15+ O 0.22490 0.68190 -0.24690
O16+ O 0.02642 0.17375 -0.15981
H*17+ H -0.01189 0.20185 -0.20746

#END