Substituted tetrazoles with *N*-oxide moiety: critical assessment of thermochemical properties

Dmitry V. Khakimov,* Leonid L. Fershtat,* and Tatyana S. Pivina
N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences,
119991 Moscow, Russian Federation.
E-mail: 7933765@mail.ru (D.V.K.), fershtat@bk.ru (L.L.F.)

Table of Contents:

S16. Optimized crystal structure coordinates for 5 polymorphs of Guanidinium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

S17. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidinium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

S18. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidinium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

S19. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidinium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

S20. Optimized crystal structure coordinates for 5 polymorphs of Ammonium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

S21. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylammonium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

S22. Optimized crystal structure coordinates for 5 polymorphs of Hydrazinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

S23. Optimized crystal structure coordinates for 5 polymorphs of Guanidinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

S24. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

S25. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

S26. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

S27. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

S28. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

S29. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

S30. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

S31. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

S32. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

S33. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

S34. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

S35. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

S36. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

S37. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

S38. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

S39. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

S40. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

S41. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

S42. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

S43. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

S44. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

S45. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

S46. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

S47. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

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 1N-oxide (Point group Cs)

C	0.00000000	0.28830200	0.00000000
N	-0.69553300	-0.90255900	0.00000000
N	-2.00495300	-0.56738300	0.00000000
N	-2.06693500	0.76549800	0.00000000
N	-0.86641400	1.31806300	0.00000000
O	-0.28280600	-2.09851400	0.00000000
N	1.40973300	0.42325500	0.00000000

O	1.87325500	1.57527700	0.00000000
O	2.10563900	-0.60025400	0.00000000

5-(trinitromethyl)tetrazolate 1N-oxide (Point group C1)

C	0.95695000	0.38962200	0.03714700
N	3.09837700	0.00236400	0.06729500
N	2.86727300	1.31382400	0.01043900
N	1.56947000	1.58750500	-0.01227900
N	1.89614000	-0.59988800	0.07888700
C	-0.46262500	0.08907200	-0.00684600
N	-1.10969100	-0.34750900	1.37404700
O	-2.32465200	-0.26499100	1.45057600
O	-0.34047000	-0.71580900	2.23452300
N	-1.28344300	1.32077500	-0.43511400
O	-1.29635600	2.22368000	0.37941200
O	-1.83367300	1.30177500	-1.52146000
N	-0.76839600	-1.09318400	-1.01095400
O	-0.24416600	-0.97417600	-2.09687000
O	-1.50812300	-1.98189500	-0.63672900
O	1.69068400	-1.85850500	0.10454200

6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (Point group C1)

C	-1.65685800	-0.30538400	-0.03718300
N	-2.31632500	-1.48145700	-0.16605200
C	-0.22317500	-0.15824900	-0.02726300
C	2.40909600	0.03545400	0.02834300
N	-3.60325700	-1.18569700	-0.12538500
N	-3.80710000	0.12230600	0.03270600
N	-2.59115600	0.70302600	0.08867400
N	0.30268100	1.08633700	-0.11048700
N	1.63014200	1.14875700	-0.08080300
N	1.80040700	-1.18677000	0.05802000
N	0.48318000	-1.31739100	0.04787400
O	-2.41742000	1.95082900	0.25144000
O	2.54870200	-2.20985900	0.10090500
O	2.22023300	2.26678600	-0.16715800
N	3.76291200	0.13913000	0.11783900
H	4.25567000	-0.71919600	-0.09885500
H	4.12744500	1.02853400	-0.20272600

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 1N-oxide (Point group Cs)

C	0.00000000	0.35341200	0.00000000
N	-0.67579800	-0.81485200	0.00000000
N	-1.97836800	-0.56092400	0.00000000
N	-2.08993200	0.75050400	0.00000000
N	-0.88518600	1.33787900	0.00000000
O	-0.19273400	-2.08588300	0.00000000
N	1.44696600	0.49773400	0.00000000
O	1.88158200	1.63617600	0.00000000
O	2.09526000	-0.54459500	0.00000000
H	-0.99663500	-2.63845300	0.00000000

5-(trinitromethyl)tetrazole 1N-oxide (Point group C1)

C	0.90289300	0.43892700	0.02274000
N	3.08462700	0.22538400	0.05875200
N	2.76477000	1.48537800	-0.01020500
N	1.41864500	1.65362700	-0.03073100
N	1.92868300	-0.43937000	0.07485200
C	-0.53225400	0.07338300	0.00667400
N	-1.06370700	-0.39073300	1.39892700
O	-2.24758900	-0.24524300	1.60085600
O	-0.22290500	-0.88570700	2.12560400
N	-1.39001700	1.28508200	-0.44495400
O	-1.44738400	2.18441600	0.36223600
O	-1.89170500	1.21216900	-1.54804700
N	-0.80515200	-1.09805000	-0.99075000

O	-0.06103900	-1.13147300	-1.95451800
O	-1.72405500	-1.84037300	-0.73091200
O	1.85965800	-1.79344500	0.16406600
H	2.09138600	-2.12584200	-0.72200200

6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (Point group C1)

C	-1.62035300	-0.37936300	-0.07839400
N	-2.29187200	-1.49444300	-0.37113700
C	-0.16178500	-0.21554000	-0.03979800
C	2.43779800	0.05668000	-0.00966500
N	-3.59779400	-1.18843700	-0.30020500
N	-3.77112900	0.06929400	0.02199200
N	-2.54742200	0.57447200	0.15649800
N	0.29802900	1.02870900	-0.20494900
N	1.62838500	1.14963100	-0.17687500
N	1.86333400	-1.18149200	0.14679700
N	0.53816600	-1.34079500	0.14362600
O	-2.34742300	1.87555600	0.51729600
O	2.62753000	-2.16495600	0.30347900
O	2.17335300	2.27430500	-0.31177800
N	3.76640800	0.19308300	0.00778000
H	4.32810500	-0.63922100	0.12686600
H	4.15118600	1.11985600	-0.11564100
H	-3.24367700	2.19931100	0.71925500

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:

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

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

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

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

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

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

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

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

S6. Optimized crystal structure coordinates for 5 polymorphs of Ammonium 5-nitrotetrazolate 1*N*-oxide (ionic form).

```
data_1a_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                12.521
_cell_length_b                10.185
_cell_length_c                8.510
_cell_angle_alpha              90.00
_cell_angle_beta               90.00
_cell_angle_gamma                90.00
_cell_volume                  1085.25
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.18148 0.45434 0.41263
H*2 H -0.12038 0.38761 0.40136
H*3 H -0.24458 0.41113 0.47002
H*4 H -0.15530 0.53395 0.47608
H*5 H -0.20566 0.48467 0.30306
C1+ C 0.48508 0.17942 0.12337
N2+ N 0.57637 0.10716 0.09612
N'3+ N 0.64454 0.18878 0.02113
N'4+ N 0.59477 0.30389 0.00547
N'5+ N 0.49768 0.30167 0.06632
O6+ O 0.59876 -0.01066 0.12978
N7+ N 0.39174 0.13341 0.19955
O8+ O 0.31649 0.21184 0.21441
O9+ O 0.38953 0.01863 0.24717

#END

data_1a_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                 8.158
_cell_length_b                 10.270
_cell_length_c                 8.314
_cell_angle_alpha               90.00
_cell_angle_beta                124.97
_cell_angle_gamma                90.00
_cell_volume                   570.805
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.31421 0.43281 0.37408
H*2 H -0.45174 0.39087 0.27744
H*3 H -0.28005 0.49343 0.29883
H*4 H -0.31774 0.48570 0.47701
H*5 H -0.20731 0.36124 0.44304
C1+ C 0.01991 0.17170 0.61430
```

```
N2+ N 0.19983 0.10809 0.69516
N'3+ N 0.31392 0.18768 0.66795
N'4+ N 0.20453 0.29333 0.57497
N'5+ N 0.02499 0.28687 0.54005
O6+ O 0.25889 -0.00134 0.77964
N7+ N -0.14613 0.12437 0.60907
O8+ O -0.29726 0.19449 0.53024
O9+ O -0.13309 0.01667 0.68239

#END

data_1a_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                 13.823
_cell_length_b                 5.049
_cell_length_c                 8.203
_cell_angle_alpha               90.00
_cell_angle_beta                104.68
_cell_angle_gamma               90.00
_cell_volume                   553.818
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.12534 0.43712 -0.25781
H*2 H -0.09645 0.26386 -0.19956
H*3 H -0.20176 0.43692 -0.27694
H*4 H -0.09549 0.59521 -0.18291
H*5 H -0.10766 0.45249 -0.37184
C1+ C -0.12598 0.96907 0.23724
N2+ N -0.03457 1.09336 0.26187
N'3+ N -0.03404 1.28688 0.37594
N'4+ N -0.12169 1.27537 0.41594
N'5+ N -0.17942 1.08444 0.33395
O6+ O 0.03784 1.04947 0.19727
N7+ N -0.15956 0.75293 0.12745
O8+ O -0.24434 0.66448 0.12046
O9+ O -0.10357 0.66335 0.04462

#END
```

```
data_1a_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                 8.047
_cell_length_b                 7.273
_cell_length_c                 9.016
_cell_angle_alpha               90.00
_cell_angle_beta                85.87
_cell_angle_gamma                 90.00
_cell_volume                   526.299
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.73910 0.21223 0.55783
H*2 H 0.77693 0.17783 0.45008
H*3 H 0.63922 0.30036 0.55822
H*4 H 0.70481 0.09526 0.61626
H*5 H 0.83544 0.27547 0.60676
C1+ C 0.25702 0.28638 0.77118
N2+ N 0.27223 0.09764 0.77619
N'3+ N 0.38537 0.06273 0.87633
N'4+ N 0.43390 0.22483 0.92743
N'5+ N 0.35837 0.36374 0.86588
O6+ O 0.20083 -0.02692 0.70625
N7+ N 0.15148 0.38561 0.68082
O8+ O 0.15309 0.55595 0.69010
O9+ O 0.06363 0.29905 0.59784

#END

data_1a_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                 14.095
_cell_length_b                 8.337
_cell_length_c                 5.098
_cell_angle_alpha               90.00
_cell_angle_beta               58.95
_cell_angle_gamma                90.00
_cell_volume                   513.23
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.02270 -0.23806 -0.31261
H*2 H -0.01470 -0.33797 -0.33742
H*3 H -0.03496 -0.17157 -0.12950
H*4 H 0.08471 -0.27285 -0.27519
H*5 H 0.05574 -0.16985 -0.50833
C1+ C -0.25740 -0.10354 0.75360
N2+ N -0.21504 -0.01396 0.89728
N'3+ N -0.30336 0.03496 1.16514
N'4+ N -0.39343 -0.02392 1.17647
N'5+ N -0.36854 -0.10872 0.93001
O6+ O -0.11610 0.02129 0.81397
N7+ N -0.19465 -0.17924 0.46472
O8+ O -0.24626 -0.25560 0.36860
O9+ O -0.09258 -0.16596 0.32323

#END
```

S7. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylammonium 5-nitrotetrazolate 1*N*-oxide (ionic form).

```
data_1b_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                 7.781
_cell_length_b                 5.374
_cell_length_c                 14.195
_cell_angle_alpha               90.00
_cell_angle_beta               97.27
_cell_angle_gamma                90.00
_cell_volume                   588.793
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.80892 0.12821 0.61944
H*2 H 0.93917 0.11551 0.61322
H*3 H 0.74551 -0.02062 0.58451
H*4 H 0.79319 0.12672 0.69061
O5 O 0.75690 0.35599 0.57617
H*6 H 0.63337 0.37539 0.58056
C1+ C 0.64625 -0.47768 0.37200
N2+ N 0.81127 -0.40829 0.35705
N'3+ N 0.84897 -0.20280 0.41059
N'4+ N 0.71126 -0.15481 0.45488
N'5+ N 0.58562 -0.31823 0.43304
O6+ O 0.91486 -0.50474 0.30561
N7+ N 0.55314 -0.68451 0.33006
O8+ O 0.40520 -0.72033 0.35138
O9+ O 0.62264 -0.81828 0.27481

#END

data_1b_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                 13.281
_cell_length_b                 6.118
_cell_length_c                 7.302
_cell_angle_alpha               90.00
_cell_angle_beta                110.55
_cell_angle_gamma               90.00
_cell_volume                   555.556
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.17197 0.94876 0.70815
H*2 H -0.23665 0.97943 0.75129
H*3 H -0.11855 1.07755 0.75176
H*4 H -0.13601 0.80438 0.77147
O5 O -0.21668 0.93220 0.50331
```

```
H*6 H -0.15767 0.90297 0.45620
C1+ C -0.08226 0.45990 0.21629
N2+ N 0.01669 0.54769 0.23634
N'3+ N 0.02023 0.74501 0.32165
N'4+ N -0.07299 0.77072 0.34999
N'5+ N -0.13722 0.60050 0.28764
O6+ O 0.09290 0.47195 0.18934
N7+ N -0.12123 0.25363 0.13360
O8+ O -0.21259 0.19958 0.12685
O9+ O -0.06316 0.13826 0.07267

#END

data_1b_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                 8.038
_cell_length_b                 9.715
_cell_length_c                 7.105
_cell_angle_alpha               90.00
_cell_angle_beta                87.41
_cell_angle_gamma                 90.00
_cell_volume                   554.257
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.35199 0.15433 0.18094
H*2 H 0.44626 0.13696 0.27165
H*3 H 0.24767 0.18790 0.25789
H*4 H 0.39120 0.22744 0.08311
O5 O 0.32535 0.02583 0.09642
H*6 H 0.23631 0.03784 0.00879
C1+ C 0.36073 0.58317 0.30532
N2+ N 0.44890 0.66335 0.42622
N'3+ N 0.55344 0.74053 0.31556
N'4+ N 0.52700 0.70649 0.13745
N'5+ N 0.41064 0.61112 0.12604
O6+ O 0.44193 0.67023 0.60422
N7+ N 0.23635 0.48589 0.35937
O8+ O 0.16905 0.42220 0.23175
O9+ O 0.20094 0.46906 0.52915
```

```
#END

data_1b_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                 8.091
_cell_length_b                 8.013
_cell_length_c                 8.978
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   582.072
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.19409 0.16042 -0.26696
H*2 H 0.07527 0.20673 -0.26872
H*3 H 0.18997 0.03538 -0.23925
H*4 H 0.24647 0.17692 -0.37084
O5 O 0.27530 0.25524 -0.15740
H*6 H 0.38911 0.21506 -0.15214
C1+ C 0.65441 0.08797 -0.11750
N2+ N 0.82177 0.07774 -0.14507
N'3+ N 0.86558 0.22683 -0.20337
N'4+ N 0.72902 0.31994 -0.20940
N'5+ N 0.59834 0.23941 -0.15808
O6+ O 0.92274 -0.04049 -0.12400
N7+ N 0.55505 -0.04016 -0.05597
O8+ O 0.40579 -0.00992 -0.03849
O9+ O 0.62076 -0.17463 -0.02289

#END

data_1b_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 12.777
_cell_length_b 10.669
_cell_length_c 8.423
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1148.2
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.20675 0.41708 -0.64664
H*2 H -0.27551 0.37137 -0.61943
H*3 H -0.14577 0.35366 -0.64105
H*4 H -0.21296 0.45477 -0.75921
O5 O -0.19756 0.51075 -0.53007
H*6 H -0.13295 0.55659 -0.55168
C1+ C 0.47614 0.17090 0.12205
N2+ N 0.56873 0.11544 0.07567
N'3+ N 0.62018 0.20263 -0.01073
N'4+ N 0.55983 0.30466 -0.01435
N'5+ N 0.47167 0.28865 0.06517
O6+ O 0.60449 0.00691 0.10252
N7+ N 0.39712 0.11389 0.21525
O8+ O 0.31833 0.17749 0.24628
O9+ O 0.41008 0.00471 0.26087

#END

S8. Optimized crystal structure coordinates for 5 polymorphs of Hydrazinium 5-nitrotetrazolate 1*N*-oxide (ionic form).

data_1c_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                 10.623
_cell_length_b                 8.965
_cell_length_c                 8.445
_cell_angle_alpha               90.00
_cell_angle_beta                46.11
_cell_angle_gamma                 90.00
_cell_volume                   579.609
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.72180 0.53916 0.15970
H*2 H 0.60583 0.55625 0.20204
H*3 H 0.73113 0.42629 0.17174
N4 N 0.71136 0.61369 0.32064
H*5 H 0.82617 0.59479 0.27884
H*6 H 0.70015 0.72549 0.30931
H*7 H 0.82343 0.57136 -0.00174
C1+ C 0.20602 0.66014 0.28998
N2+ N 0.24540 0.51004 0.25453
N'3+ N 0.37545 0.49182 0.24762
N'4+ N 0.41018 0.62606 0.27787
N'5+ N 0.30960 0.73097 0.30417
O6+ O 0.18075 0.40393 0.23140
N7+ N 0.07676 0.73062 0.30893
O8+ O 0.05829 0.86742 0.34087
O9+ O -0.01070 0.65358 0.29298

#END

data_1c_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                 7.589
_cell_length_b                 7.343
_cell_length_c                 5.525
_cell_angle_alpha               90.00
_cell_angle_beta                80.66
_cell_angle_gamma                 90.00
_cell_volume                   303.805
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.71115 0.60292 -0.43047
H*2 H 0.58738 0.64186 -0.34092
H*3 H 0.80286 0.68554 -0.36631
N4 N 0.71878 0.63934 -0.68957
H*5 H 0.84270 0.60223 -0.77676
H*6 H 0.62599 0.55831 -0.75122
H*7 H 0.73414 0.46980 -0.38393
C1+ C -0.25985 0.07499 0.17708
N2+ N -0.08133 0.07333 0.19850
N'3+ N -0.06733 0.17439 0.39897
N'4+ N -0.23126 0.23242 0.49031
N'5+ N -0.35157 0.17453 0.35994
O6+ O 0.05052 -0.00261 0.06755
N7+ N -0.33690 -0.01377 -0.00794
O8+ O -0.50066 0.00182 0.00006
O9+ O -0.23869 -0.10166 -0.16702

#END

data_1c_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                 13.219
_cell_length_b                 6.563
_cell_length_c                 7.074
_cell_angle_alpha               90.00
_cell_angle_beta               111.42
_cell_angle_gamma                90.00
_cell_volume                   571.324
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.32704 0.46933 0.29644
H*2 H -0.37304 0.35238 0.21057
H*3 H -0.26125 0.48634 0.25303
N4 N -0.28740 0.40699 0.50735
H*5 H -0.24084 0.52295 0.59130
H*6 H -0.35326 0.38823 0.54860
```

H*7 H -0.37246 0.60162 0.26223
C1+ C -0.07621 0.44121 0.21933
N2+ N 0.02401 0.51546 0.23418
N'3+ N 0.02888 0.70821 0.30428
N'4+ N -0.06482 0.74439 0.32913
N'5+ N -0.13061 0.58534 0.27892
O6+ O 0.10023 0.43231 0.19427
N7+ N -0.11682 0.24388 0.15197
O8+ O -0.20917 0.20176 0.14793
O9+ O -0.05912 0.12407 0.10090

#END

data_1c_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 7.228
_cell_length_b 14.074
_cell_length_c 6.020
_cell_angle_alpha 90.00
_cell_angle_beta 90.92
_cell_angle_gamma 90.00
_cell_volume 612.317
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.73667 -0.91676 -0.26283
H*2 H 0.63432 -0.88623 -0.16989
H*3 H 0.69472 -0.98515 -0.29674
N4 N 0.90357 -0.92130 -0.12692
H*5 H 1.00388 -0.95265 -0.21950
H*6 H 0.94313 -0.85316 -0.09194
H*7 H 0.74672 -0.88008 -0.41074
C1+ C 0.18114 0.66298 0.66559
N2+ N 0.14021 0.75254 0.74372
N'3+ N 0.04704 0.73917 0.93409
N'4+ N 0.03439 0.64554 0.96521
N'5+ N 0.11444 0.59708 0.80511
O6+ O 0.17639 0.83375 0.66541
N7+ N 0.27835 0.64237 0.46896
O8+ O 0.30338 0.55737 0.42290

```
O9+ O 0.33315 0.70917 0.35359

#END

data_1c_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                 22.845
_cell_length_b                 5.548
_cell_length_c                 14.747
_cell_angle_alpha               90.00
_cell_angle_beta               139.55
_cell_angle_gamma                90.00
_cell_volume                   1212.64
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.38149 0.06041 0.72057
H*2 H 0.43594 -0.02865 0.81211
H*3 H 0.37804 0.01033 0.64943
N4 N 0.39965 0.31668 0.74570
H*5 H 0.34575 0.40362 0.65396
H*6 H 0.40398 0.36442 0.81757
H*7 H 0.32362 0.00298 0.68483
C1+ C 0.63416 -0.44767 0.06009
N2+ N 0.65052 -0.34949 -0.00495
N'3+ N 0.59706 -0.15277 -0.07393
N'4+ N 0.55146 -0.13738 -0.04988
N'5+ N 0.57236 -0.31378 0.03121
O6+ O 0.70302 -0.41653 -0.00583
N7+ N 0.67551 -0.65717 0.14464
O8+ O 0.65289 -0.72095 0.19542
O9+ O 0.73157 -0.76562 0.16377

#END
```

S9. Optimized crystal structure coordinates for 5 polymorphs of Guanidinium 5-nitrotetrazolate 1*N*-oxide (ionic form).

```
data_1d_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                 6.065
_cell_length_b                 7.519
_cell_length_c                 15.109
_cell_angle_alpha               90.00
_cell_angle_beta                90.19
_cell_angle_gamma                 90.00
_cell_volume                   689.008
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25006 0.17437 -0.22862
N2 N 0.24994 0.18343 -0.14022
H*3 H 0.24990 0.07228 -0.10262
H*4 H 0.24990 0.30169 -0.10844
N5 N 0.25012 0.01601 -0.26891
H*6 H 0.25021 0.00615 -0.33562
H*7 H 0.25008 -0.09842 -0.23383
N8 N 0.25012 0.32367 -0.27672
H*9 H 0.25008 0.44467 -0.24762
H*10 H 0.25021 0.31984 -0.34358
C1+ C 0.24997 0.77134 -0.01429
N2+ N 0.24998 0.58794 -0.01424
N'3+ N 0.25002 0.53851 -0.10025
N'4+ N 0.25003 0.68737 -0.14833
N'5+ N 0.25001 0.83140 -0.09820
O6+ O 0.24995 0.47835 0.04929
N7+ N 0.24994 0.88147 0.06174
O8+ O 0.24994 1.04485 0.04974
O9+ O 0.24991 0.81069 0.13570

#END

data_1d_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                   6.226
_cell_length_b                   7.541
_cell_length_c                   7.604
_cell_angle_alpha                 82.24
_cell_angle_beta                 79.69
_cell_angle_gamma                   79.70
_cell_volume                     343.622
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.24336 0.29182 0.47724
N2 N -0.24044 0.42883 0.57116
H*3 H -0.23535 0.40801 0.70454
H*4 H -0.24322 0.55719 0.51148
N5 N -0.23955 0.12329 0.55974
H*6 H -0.24165 0.01782 0.49133
H*7 H -0.23445 0.09648 0.69291
N8 N -0.25010 0.32334 0.30082
H*9 H -0.25307 0.44963 0.23585
H*10 H -0.25241 0.22179 0.22734
C1+ C 0.25063 0.23307 -0.05442
N2+ N 0.25332 0.04952 -0.05231
N'3+ N 0.24199 0.02274 -0.22240
N'4+ N 0.23307 0.18438 -0.31940
N'5+ N 0.23799 0.31529 -0.22153
O6+ O 0.26383 -0.07689 0.07494
N7+ N 0.25968 0.32322 0.09521
O8+ O 0.25561 0.48987 0.06959
O9+ O 0.27108 0.23289 0.24269

#END

data_1d_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                 13.281
_cell_length_b                 7.548
_cell_length_c                 15.032
_cell_angle_alpha               90.00
_cell_angle_beta               113.83
_cell_angle_gamma                90.00
_cell_volume                   1378.42
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.62691 0.57364 0.23013
N2 N 0.62891 0.56534 0.31969
H*3 H 0.62802 0.44782 0.35158
H*4 H 0.63137 0.67635 0.35811
N5 N 0.62367 0.42455 0.18097
H*6 H 0.62211 0.42781 0.11322
H*7 H 0.62267 0.30427 0.21014
N8 N 0.62816 0.73103 0.18972
H*9 H 0.63060 0.84528 0.22559
H*10 H 0.62669 0.74030 0.12215
C1+ C 0.12580 0.52252 -0.05701
N2+ N 0.12325 0.33985 -0.05806
N'3+ N 0.12845 0.29076 -0.14257
N'4+ N 0.13381 0.43910 -0.18875
N'5+ N 0.13238 0.58247 -0.13881
O6+ O 0.11737 0.23060 0.00350
N7+ N 0.12212 0.63210 0.01809
O8+ O 0.12521 0.79483 0.00731
O9+ O 0.11607 0.56148 0.09008

#END

data_1d_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                 7.560
_cell_length_b                 7.587
_cell_length_c                 7.576
_cell_angle_alpha               66.03
```

```
_cell_angle_beta                60.62
_cell_angle_gamma               82.33
_cell_volume                    344.813
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.37364 0.45970 -0.75323
N2 N -0.40085 0.63922 -0.75840
H*3 H -0.52552 0.70573 -0.75973
H*4 H -0.29754 0.71360 -0.76112
N5 N -0.51291 0.36466 -0.74971
H*6 H -0.49534 0.22894 -0.74579
H*7 H -0.63977 0.42580 -0.75088
N8 N -0.20716 0.37522 -0.75158
H*9 H -0.10005 0.44443 -0.75417
H*10 H -0.18361 0.23970 -0.74769
C1+ C -0.15319 0.11895 0.75140
N2+ N 0.03135 0.11841 0.74715
N'3+ N 0.05494 0.28701 0.75721
N'4+ N -0.10944 0.38167 0.76690
N'5+ N -0.23911 0.28369 0.76371
O6+ O 0.16093 -0.00649 0.73635
N7+ N -0.24088 -0.02992 0.74404
O8+ O -0.40890 -0.00598 0.74938
O9+ O -0.14718 -0.17516 0.73278

#END

data_1d_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                  11.386
_cell_length_b                  9.983
_cell_length_c                  6.625
_cell_angle_alpha               90.00
_cell_angle_beta                67.17
_cell_angle_gamma               90.00
_cell_volume                    694.047
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.16537 0.58513 0.44751
N2 N 0.08977 0.48218 0.44953
H*3 H -0.00013 0.49705 0.45958
H*4 H 0.12032 0.38651 0.44107
N5 N 0.12240 0.71073 0.45891
H*6 H 0.17794 0.78995 0.45762
H*7 H 0.03314 0.73007 0.46914
N8 N 0.28394 0.56248 0.43409
H*9 H 0.31831 0.46838 0.42533
H*10 H 0.34264 0.63880 0.43232
C1+ C 0.18965 0.13851 0.44662
N2+ N 0.27793 0.04751 0.45831
N'3+ N 0.37910 0.12062 0.45254
N'4+ N 0.35066 0.24899 0.43808
N'5+ N 0.23620 0.26351 0.43410
O6+ O 0.27355 -0.07894 0.47187
N7+ N 0.06822 0.10682 0.44749
O8+ O 0.00034 0.20145 0.43584
O9+ O 0.03578 -0.01221 0.45966

#END
```

S10. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidinium 5-nitrotetrazolate 1*N*-oxide (ionic form).

```
data_1e_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                 4.008
_cell_length_b                 15.380
_cell_length_c                 12.917
_cell_angle_alpha               90.00
_cell_angle_beta                90.45
_cell_angle_gamma                 90.00
_cell_volume                   796.219
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

C1 C 0.10075 -0.19812 -0.10654
N2 N 0.21170 -0.11993 -0.07613
H*3 H 0.37608 -0.11365 -0.01689
H*4 H 0.13377 -0.06500 -0.11170
N5 N 0.21079 -0.26978 -0.05707
H*6 H 0.37591 -0.26392 0.00248
N7 N -0.11558 -0.20632 -0.18450
H*8 H -0.20373 -0.15412 -0.22345
H*9 H -0.19148 -0.26701 -0.20437
N10 N 0.09401 -0.35127 -0.08919
H*11 H 0.28746 -0.38887 -0.11346
H*12 H -0.02870 -0.38122 -0.03035
C1+ C 0.19536 0.43467 0.14724
N2+ N 0.28995 0.49456 0.22131
N'3+ N 0.15634 0.57119 0.19087
N'4+ N -0.00928 0.55635 0.10261
N'5+ N 0.00923 0.47405 0.07383
O6+ O 0.46394 0.48569 0.30277
N7+ N 0.27924 0.34522 0.14732
O8+ O 0.17286 0.30028 0.07433
O9+ O 0.45250 0.31635 0.21922

#END

data_1e_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 17.892
_cell_length_b 12.917
_cell_length_c 3.916
_cell_angle_alpha 90.00
_cell_angle_beta 119.68
_cell_angle_gamma 90.00
_cell_volume 786.295
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.76411 0.54148 0.85667
N2 N 0.74231 0.63574 0.69383
H*3 H 0.68021 0.65861 0.54292
H*4 H 0.78750 0.68665 0.71758

N5 N 0.70191 0.47590 0.81824
H*6 H 0.63940 0.49839 0.66703
N7 N 0.84586 0.51146 1.05520
H*8 H 0.89428 0.55844 1.09029
H*9 H 0.85882 0.43929 1.17255
N10 N 0.72508 0.37754 0.98898
H*11 H 0.70596 0.36827 1.19261
H*12 H 0.69837 0.32177 0.77837
C1+ C -0.02540 0.20909 0.92184
N2+ N 0.04615 0.27077 1.03941
N'3+ N 0.01971 0.35246 0.79118
N'4+ N -0.06390 0.33872 0.53945
N'5+ N -0.09342 0.25234 0.61036
O6+ O 0.12266 0.25960 1.31632
N7+ N -0.02793 0.11451 1.09875
O8+ O -0.09802 0.06861 0.95509
O9+ O 0.03898 0.08240 1.38471

#END

data_1e_3
_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 4.179
_cell_length_b 23.731
_cell_length_c 10.362
_cell_angle_alpha 90.00
_cell_angle_beta 131.27
_cell_angle_gamma 90.00
_cell_volume 772.368
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.37155 -0.11092 -0.16591
N2 N 0.34436 -0.07582 -0.27410
H*3 H 0.35077 -0.09033 -0.36405
H*4 H 0.31664 -0.03379 -0.26865
N5 N 0.40817 -0.16668 -0.17741
H*6 H 0.41480 -0.18153 -0.26747
N7 N 0.36308 -0.09178 -0.04758
H*8 H 0.33597 -0.05027 -0.03503

H*9 H 0.38475 -0.12016 0.03106
N10 N 0.43644 -0.20313 -0.06405
H*11 H 0.18781 -0.23069 -0.13046
H*12 H 0.71777 -0.22446 0.00877
C1+ C -0.14753 0.61617 -0.10038
N2+ N -0.12345 0.65639 -0.18975
N'3+ N -0.08748 0.70644 -0.11885
N'4+ N -0.09056 0.69568 0.00672
N'5+ N -0.12667 0.64123 0.02151
O6+ O -0.13083 0.65149 -0.31328
N7+ N -0.18806 0.55735 -0.13070
O8+ O -0.20541 0.52697 -0.03788
O9+ O -0.20411 0.53918 -0.24683

#END

data_1e_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 4.050
_cell_length_b 11.568
_cell_length_c 21.277
_cell_angle_alpha 90.00
_cell_angle_beta 128.27
_cell_angle_gamma 90.00
_cell_volume 782.617
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.88871 0.21257 0.34858
N2 N 0.88465 0.15940 0.29216
H*3 H 0.87406 0.20474 0.25035
H*4 H 0.89210 0.07230 0.28989
N5 N 0.87845 0.32887 0.34953
H*6 H 0.86779 0.37492 0.30771
N7 N 0.90266 0.15283 0.40357
H*8 H 0.91066 0.06557 0.40480
H*9 H 0.90513 0.19737 0.44492
N10 N 0.88275 0.38393 0.40861
H*11 H 1.14164 0.43528 0.44304
H*12 H 0.61636 0.43166 0.38298

```
C1+ C 0.85795 0.24886 0.13181
N2+ N 0.91880 0.32615 0.09048
N'3+ N 1.01624 0.42808 0.12940
N'4+ N 1.01209 0.41063 0.19090
N'5+ N 0.91704 0.30264 0.19417
O6+ O 0.89534 0.31246 0.02882
N7+ N 0.74975 0.13075 0.11236
O8+ O 0.70681 0.07318 0.15614
O9+ O 0.70359 0.09087 0.05338

#END

data_1e_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                 4.198
_cell_length_b                 23.686
_cell_length_c                 10.393
_cell_angle_alpha               90.00
_cell_angle_beta                48.50
_cell_angle_gamma                 90.00
_cell_volume                   773.983
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.76045 0.63819 0.18067
N2 N 0.78924 0.67286 0.07149
H*3 H 0.78674 0.65786 -0.01885
H*4 H 0.81428 0.71506 0.07655
N5 N 0.72753 0.58218 0.16967
H*6 H 0.72484 0.56684 0.07922
N7 N 0.76376 0.65797 0.29951
H*8 H 0.78799 0.69968 0.31173
H*9 H 0.74110 0.62988 0.37891
N10 N 0.69756 0.54617 0.28407
H*11 H 0.41770 0.52452 0.35663
H*12 H 0.94741 0.51879 0.21844
C1+ C 0.79117 -0.13395 0.24329
N2+ N 0.78041 -0.09440 0.14884
N'3+ N 0.76234 -0.04356 0.21250
N'4+ N 0.76261 -0.05323 0.33891
```

```
N'5+ N 0.77990 -0.10772 0.36111
O6+ O 0.78517 -0.10043 0.02662
N7+ N 0.81104 -0.19323 0.22121
O8+ O 0.81852 -0.22287 0.31773
O9+ O 0.81992 -0.21250 0.10817

#END
```

S11. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidinium 5-nitrotetrazolate 1*N*-oxide (ionic form).

```
data_1f_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                 6.911
_cell_length_b                 12.572
_cell_length_c                 13.119
_cell_angle_alpha               141.77
_cell_angle_beta                114.09
_cell_angle_gamma                42.63
_cell_volume                   436.759
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.04567 0.29695 0.26641
N2 N 0.25022 0.13537 0.24039
H*3 H 0.40165 0.11127 0.20978
N4 N -0.12917 0.41913 0.25116
H*5 H -0.35280 0.54190 0.27063
N6 N -0.25444 0.33609 0.30687
H*7 H -0.18121 0.24008 0.31696
H*8 H -0.47892 0.45680 0.32716
N9 N 0.09628 0.37344 0.20848
N10 N 0.33566 0.00889 0.25643
H*11 H 0.41445 0.05388 0.35616
H*12 H 0.12479 0.30023 0.09004
H*13 H 0.03299 0.53648 0.30908
H*14 H 0.50604 -0.18182 0.13764
C1+ C -0.15050 0.14733 0.70589
N2+ N 0.05710 0.09393 0.77909
N'3+ N -0.02663 0.31045 0.93431
N'4+ N -0.27312 0.48274 0.95055
N'5+ N -0.35468 0.39001 0.81406
```

```
O6+ O 0.28426 -0.10847 0.72280
N7+ N -0.15165 -0.02479 0.54214
O8+ O -0.35599 0.05490 0.49578
O9+ O 0.04852 -0.24388 0.45393

#END

data_1f_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                 8.366
_cell_length_b                 8.871
_cell_length_c                 6.650
_cell_angle_alpha               110.30
_cell_angle_beta                76.78
_cell_angle_gamma               93.20
_cell_volume                   450.459
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24334 0.52410 0.00180
N2 N 0.28552 0.38137 -0.15668
H*3 H 0.31872 0.37896 -0.31469
N4 N 0.24661 0.65670 -0.05399
H*5 H 0.21486 0.76536 0.06493
N6 N 0.19873 0.53454 0.21189
H*7 H 0.19807 0.43168 0.24619
H*8 H 0.16636 0.64057 0.33458
N9 N 0.29410 0.64129 -0.27637
N10 N 0.28187 0.24392 -0.09767
H*11 H 0.39609 0.19151 -0.14721
H*12 H 0.20100 0.67884 -0.32442
H*13 H 0.39628 0.70591 -0.30266
H*14 H 0.20127 0.16450 -0.16892
C1+ C -0.18242 -0.06221 0.71123
N2+ N -0.09103 -0.20402 0.61426
N'3+ N 0.06433 -0.16452 0.63450
N'4+ N 0.06316 -0.00604 0.73908
N'5+ N -0.08485 0.06000 0.78819
O6+ O -0.13294 -0.34612 0.52210
N7+ N -0.35290 -0.04578 0.72846
O8+ O -0.41612 0.09134 0.82127
O9+ O -0.43000 -0.16730 0.65119
```

```
#END

data_1f_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                 12.865
_cell_length_b                 8.143
_cell_length_c                 8.958
_cell_angle_alpha               90.00
_cell_angle_beta               109.15
_cell_angle_gamma                90.00
_cell_volume                   886.507
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74309 -0.16055 -0.02577
N2 N 0.82160 -0.17189 0.11556
H*3 H 0.90117 -0.17412 0.11808
N4 N 0.77242 -0.15268 -0.15689
H*5 H 0.71353 -0.14407 -0.26449
N6 N 0.63736 -0.15711 -0.03630
H*7 H 0.61913 -0.16333 0.06542
H*8 H 0.57655 -0.14862 -0.14130
N9 N 0.88430 -0.15660 -0.14145
N10 N 0.79060 -0.18003 0.25147
H*11 H 0.82302 -0.08308 0.32351
H*12 H 0.90088 -0.25604 -0.19875
H*13 H 0.90611 -0.05151 -0.18516
H*14 H 0.81779 -0.28713 0.30995
C1+ C -0.10502 0.34299 0.55844
N2+ N -0.05541 0.41869 0.70198
N'3+ N -0.06424 0.58181 0.67266
N'4+ N -0.11689 0.60007 0.51819
N'5+ N -0.14290 0.45739 0.44513
O6+ O -0.00939 0.35854 0.83794
N7+ N -0.11518 0.17133 0.53238
O8+ O -0.16245 0.12375 0.39507
O9+ O -0.07696 0.07787 0.64622

#END
```

```
data_1f_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                 13.033
_cell_length_b                 8.446
_cell_length_c                 8.795
_cell_angle_alpha               90.00
_cell_angle_beta                77.05
_cell_angle_gamma               90.00
_cell_volume                   943.501
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.49774 0.75208 -0.52609
N2 N 0.42345 0.78400 -0.39788
H*3 H 0.34954 0.80720 -0.41169
N4 N 0.47180 0.75204 -0.66609
H*5 H 0.52755 0.72798 -0.76388
N6 N 0.59602 0.72079 -0.51507
H*7 H 0.61195 0.72213 -0.40739
H*8 H 0.65353 0.69635 -0.60981
N9 N 0.36777 0.78543 -0.67335
N10 N 0.45089 0.78387 -0.25265
H*11 H 0.40792 0.70079 -0.18189
H*12 H 0.36513 0.88388 -0.73916
H*13 H 0.33576 0.69152 -0.71866
H*14 H 0.43722 0.89271 -0.20234
C1+ C 0.13505 0.80323 -0.03976
N2+ N 0.17608 0.89674 -0.16746
N'3+ N 0.16988 1.04732 -0.11418
N'4+ N 0.12694 1.04144 0.03843
N'5+ N 0.10478 0.89488 0.08757
O6+ O 0.21334 0.86004 -0.30851
N7+ N 0.12568 0.63621 -0.04063
O8+ O 0.08673 0.57035 0.08532
O9+ O 0.15635 0.56453 -0.16529

#END

data_1f_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                 16.653
_cell_length_b                 6.623
_cell_length_c                 16.250
_cell_angle_alpha               90.00
_cell_angle_beta                93.68
_cell_angle_gamma                 90.00
_cell_volume                   1788.56
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.01161 0.40785 0.62704
N2 N -0.06117 0.33101 0.60593
H*3 H -0.06402 0.18499 0.58668
N4 N 0.07712 0.29009 0.62195
H*5 H 0.13251 0.34697 0.63780
N6 N 0.01901 0.59839 0.65273
H*7 H -0.03190 0.68138 0.65558
H*8 H 0.07313 0.66009 0.66901
N9 N 0.06712 0.09056 0.59470
N10 N -0.12906 0.45417 0.61135
H*11 H -0.16664 0.39283 0.65160
H*12 H 0.09631 0.06845 0.54228
H*13 H 0.08808 -0.00729 0.63938
H*14 H -0.15843 0.46839 0.55473
C1+ C 0.78245 0.09424 0.16072
N2+ N 0.85366 0.10388 0.20880
N'3+ N 0.83314 0.15180 0.28553
N'4+ N 0.75317 0.16928 0.28211
N'5+ N 0.72041 0.13528 0.20716
O6+ O 0.92552 0.07618 0.19045
N7+ N 0.77480 0.04837 0.07546
O8+ O 0.70585 0.04609 0.04149
O9+ O 0.83641 0.01314 0.03920

#END
```

S12. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidinium 5-nitrotetrazolate 1*N*-oxide (ionic form).

```
data_1g_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                 8.542
_cell_length_b                 8.669
_cell_length_c                 13.409
_cell_angle_alpha               90.00
_cell_angle_beta                79.18
_cell_angle_gamma                 90.00
_cell_volume                   975.292
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.50934 -0.38924 -0.23794
N2 N 0.48843 -0.41516 -0.33313
H*3 H 0.37497 -0.41388 -0.34613
N4 N 0.65655 -0.38966 -0.21667
H*5 H 0.74914 -0.41008 -0.27482
N6 N 0.38303 -0.36291 -0.16401
H*7 H 0.40391 -0.34377 -0.09287
N8 N 0.67522 -0.36226 -0.11658
N9 N 0.62239 -0.44238 -0.40904
H*10 H 0.62996 -0.36033 -0.46409
H*11 H 0.72793 -0.45491 -0.08983
H*12 H 0.74346 -0.26657 -0.11387
H*13 H 0.61443 -0.54867 -0.44004
N14 N 0.23041 -0.36308 -0.18821
H*15 H 0.16236 -0.44665 -0.14788
H*16 H 0.17790 -0.25831 -0.17192
C1+ C 0.04623 -0.34859 0.61579
N2+ N 0.17298 -0.25851 0.57070
N'3+ N 0.11887 -0.11165 0.57714
N'4+ N -0.03329 -0.11631 0.62412
N'5+ N -0.08135 -0.25854 0.64868
O6+ O 0.31388 -0.29518 0.53004
N7+ N 0.04816 -0.51107 0.62642
O8+ O -0.07702 -0.57426 0.66916
```

```
O9+ O 0.17294 -0.58166 0.59304

#END

data_1g_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                 12.097
_cell_length_c                 7.278
_cell_angle_alpha               66.14
_cell_angle_beta                99.88
_cell_angle_gamma               134.68
_cell_volume                   489.913
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24995 -0.26274 0.97674
N2 N 0.16090 -0.22875 0.82305
H*3 H 0.22320 -0.18832 0.67941
N4 N 0.17390 -0.31646 1.16914
H*5 H 0.04858 -0.32979 1.19208
N6 N 0.41505 -0.24301 0.93803
H*7 H 0.47807 -0.27011 1.05873
N8 N 0.26976 -0.35113 1.32707
N9 N -0.01149 -0.25039 0.86752
H*10 H -0.14843 -0.33835 0.82080
H*11 H 0.33546 -0.27458 1.40184
H*12 H 0.15455 -0.47523 1.42679
H*13 H 0.03249 -0.13769 0.79584
N14 N 0.49158 -0.18670 0.73563
H*15 H 0.65327 -0.07496 0.69511
H*16 H 0.47236 -0.27562 0.72006
C1+ C -0.25055 0.70947 0.26023
N2+ N -0.06553 0.76939 0.34803
N'3+ N 0.03415 0.92320 0.33320
N'4+ N -0.08820 0.95143 0.24044
N'5+ N -0.26255 0.82409 0.19394
O6+ O 0.00825 0.70357 0.42892
N7+ N -0.40570 0.55176 0.24154
O8+ O -0.56358 0.51752 0.15798
O9+ O -0.37711 0.45657 0.30851
```

```
#END

data_1g_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                 17.174
_cell_length_b                 8.077
_cell_length_c                 7.328
_cell_angle_alpha               90.00
_cell_angle_beta                73.54
_cell_angle_gamma                90.00
_cell_volume                   974.841
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.51128 0.73424 0.46668
N2 N 0.50778 0.73227 0.28625
H*3 H 0.45234 0.74586 0.26394
N4 N 0.58288 0.71682 0.50399
H*5 H 0.63309 0.70241 0.39156
N6 N 0.44318 0.75364 0.60980
H*7 H 0.44840 0.75445 0.74454
N8 N 0.58492 0.71931 0.69379
N9 N 0.57982 0.71182 0.13921
H*10 H 0.58928 0.81196 0.05121
H*11 H 0.60746 0.61024 0.72674
H*12 H 0.62034 0.81464 0.71426
H*13 H 0.57640 0.60756 0.06370
N14 N 0.36910 0.77159 0.56704
H*15 H 0.33066 0.67831 0.62833
H*16 H 0.34354 0.88271 0.61584
C1+ C 0.28675 0.79746 0.20843
N2+ N 0.35428 0.87877 0.09762
N'3+ N 0.33521 1.04154 0.11096
N'4+ N 0.25959 1.05420 0.22503
N'5+ N 0.22829 0.90820 0.28685
O6+ O 0.42214 0.82337 -0.00050
N7+ N 0.27915 0.62409 0.23676
O8+ O 0.21382 0.57126 0.34147
O9+ O 0.33724 0.53441 0.15685
```

```
#END

data_1g_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                 8.083
_cell_length_b                 8.880
_cell_length_c                 7.310
_cell_angle_alpha               71.35
_cell_angle_beta                90.13
_cell_angle_gamma               94.17
_cell_volume                   495.7
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74936 0.52899 -0.03137
N2 N 0.74150 0.66518 0.00940
H*3 H 0.73670 0.76753 -0.10342
N4 N 0.75593 0.39063 0.11207
H*5 H 0.75468 0.39404 0.24973
N6 N 0.75065 0.53116 -0.21557
H*7 H 0.75670 0.42540 -0.24042
N8 N 0.76408 0.24993 0.06566
N9 N 0.74032 0.65971 0.20310
H*10 H 0.63393 0.70179 0.23506
H*11 H 0.87037 0.19800 0.11698
H*12 H 0.66408 0.17305 0.12423
H*13 H 0.84022 0.72673 0.22781
N14 N 0.74369 0.67732 -0.36286
H*15 H 0.84693 0.69965 -0.44978
H*16 H 0.64063 0.67471 -0.44252
C1+ C 0.26378 -0.07021 0.28178
N2+ N 0.34200 -0.20480 0.37981
N'3+ N 0.50647 -0.16250 0.35425
N'4+ N 0.52305 -0.00939 0.24567
N'5+ N 0.37799 0.05049 0.19900
O6+ O 0.28289 -0.34322 0.47675
N7+ N 0.09001 -0.05886 0.26888
O8+ O 0.04027 0.07195 0.17434
O9+ O -0.00304 -0.17833 0.35138

#END
```

```
data_1g_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                 8.373
_cell_length_b                 8.966
_cell_length_c                 13.186
_cell_angle_alpha               90.00
_cell_angle_beta                83.05
_cell_angle_gamma                 90.00
_cell_volume                   982.63
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74342 -0.49133 0.51334
N2 N 0.74775 -0.53416 0.61038
H*3 H 0.74505 -0.64543 0.62528
N4 N 0.74669 -0.34590 0.48952
H*5 H 0.75247 -0.27165 0.54722
N6 N 0.73582 -0.59393 0.44012
H*7 H 0.73274 -0.55691 0.36752
N8 N 0.74204 -0.30403 0.38754
N9 N 0.75568 -0.42475 0.68549
H*10 H 0.85796 -0.43803 0.71920
H*11 H 0.64303 -0.24010 0.38168
H*12 H 0.84311 -0.24560 0.36166
H*13 H 0.65788 -0.43253 0.73923
N14 N 0.73254 -0.74521 0.46699
H*15 H 0.62924 -0.79311 0.44915
H*16 H 0.82931 -0.79861 0.42912
C1+ C -0.23384 0.50718 0.13161
N2+ N -0.15305 0.40019 0.18066
N'3+ N 0.00255 0.44393 0.17072
N'4+ N 0.01171 0.57129 0.11798
N'5+ N -0.12978 0.61299 0.09297
O6+ O -0.20358 0.28269 0.22706
N7+ N -0.40069 0.50726 0.12263
O8+ O -0.45404 0.61266 0.07572
O9+ O -0.48453 0.40359 0.16146

#END
```

S13. Optimized crystal structure coordinates for 5 polymorphs of Ammonium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

```
data_2a_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                 9.441
_cell_length_b                 9.765
_cell_length_c                 9.110
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   839.863
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.33844 0.67007 -0.07646
H*2 H 0.36393 0.73600 -0.16035
H*3 H 0.23262 0.64591 -0.08222
H*4 H 0.39771 0.58221 -0.08586
H*5 H 0.35950 0.71616 0.02259
C1+ C 0.12926 0.12627 0.79447
N'2+ N -0.08324 0.03989 0.79603
N'3+ N -0.06705 0.12280 0.68103
N'4+ N 0.06143 0.17764 0.67671
N5+ N 0.04021 0.04138 0.86964
C6+ C 0.27149 0.15511 0.84652
N7+ N 0.38441 0.03763 0.81885
O8+ O 0.50865 0.07152 0.82540
O9+ O 0.33743 -0.07521 0.79265
N10+ N 0.33476 0.28127 0.76892
O11+ O 0.35983 0.26442 0.63924
O12+ O 0.35370 0.38501 0.84050
N13+ N 0.27316 0.18156 1.01772
O14+ O 0.18369 0.26126 1.06007
O15+ O 0.36343 0.12427 1.09035
O16+ O 0.06660 -0.02330 0.98816

#END

data_2a_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                   9.057
_cell_length_b                   10.934
_cell_length_c                   8.797
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
_cell_angle_gamma                    90.00
_cell_volume                     871.16
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.49731 0.23543 -0.12389
H*2 H -0.40320 0.26722 -0.17587
H*3 H -0.56043 0.30824 -0.08869
H*4 H -0.55669 0.18333 -0.19952
H*5 H -0.46893 0.18294 -0.03147
C1+ C -0.11406 0.04204 0.62543
N'2+ N -0.34736 0.02038 0.67826
N'3+ N -0.29501 -0.08091 0.61344
N'4+ N -0.15286 -0.07088 0.57931
N5+ N -0.23407 0.09962 0.68613
C6+ C 0.02750 0.10330 0.61139
N7+ N 0.11999 0.11433 0.76390
O8+ O 0.25159 0.13520 0.74948
O9+ O 0.05208 0.10025 0.88125
N10+ N 0.13092 0.03423 0.50196
O11+ O 0.17271 -0.06454 0.54875
O12+ O 0.16150 0.08173 0.38076
N13+ N 0.00827 0.23872 0.55161
O14+ O -0.07111 0.24825 0.44138
O15+ O 0.07544 0.31949 0.61663
O16+ O -0.24007 0.20824 0.73866

#END

data_2a_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                 10.519
_cell_length_b                 9.133
_cell_length_c                 9.046
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   869.049
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.73922 0.87850 0.51538
H*2 H 0.80840 0.89633 0.43719
H*3 H 0.67556 0.80228 0.47654
H*4 H 0.78048 0.84041 0.61092
H*5 H 0.69244 0.97498 0.53687
C1+ C 0.04471 0.86743 -0.88899
N'2+ N 0.02810 0.80981 -0.65634
N'3+ N -0.07814 0.87450 -0.70303
N'4+ N -0.07131 0.91150 -0.84461
N5+ N 0.10737 0.80501 -0.77286
C6+ C 0.10467 0.88469 -1.03247
N7+ N 0.11278 0.74052 -1.12980
O8+ O 0.13105 0.75814 -1.26180
O9+ O 0.09927 0.62562 -1.06473
N10+ N 0.03080 0.99361 -1.13017
O11+ O -0.07319 0.95051 -1.16961
O12+ O 0.08004 1.11086 -1.15904
N13+ N 0.24622 0.94069 -1.01661
O14+ O 0.25888 1.04440 -0.93439
O15+ O 0.32797 0.87949 -1.08870
O16+ O 0.22006 0.75347 -0.77246

#END

data_2a_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 11.143
_cell_length_b 9.217
_cell_length_c 8.657
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 889.117
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.26326 0.12041 -0.46812
H*2 H -0.28542 0.13147 -0.58277
H*3 H -0.33542 0.07930 -0.40852
H*4 H -0.19164 0.05083 -0.45768
H*5 H -0.24056 0.22004 -0.42351
C1+ C 0.03191 0.87877 0.59007
N'2+ N -0.00081 0.84406 0.83514
N'3+ N -0.10014 0.89195 0.76617
N'4+ N -0.08341 0.91463 0.61640
N5+ N 0.08409 0.83568 0.72513
C6+ C 0.09977 0.88733 0.44722
N7+ N 0.12534 0.73680 0.36473
O8+ O 0.15314 0.74261 0.22855
O9+ O 0.11423 0.62923 0.44386
N10+ N 0.03247 0.97679 0.32432
O11+ O -0.05849 0.91986 0.27585
O12+ O 0.07360 1.09400 0.28670
N13+ N 0.22715 0.95840 0.47444
O14+ O 0.22495 1.06982 0.54867
O15+ O 0.31400 0.89941 0.41729
O16+ O 0.19277 0.79666 0.74553

#END

data_2a_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 10.295
_cell_length_b 10.251

_cell_length_c 8.579
_cell_angle_alpha 90.00
_cell_angle_beta 72.60
_cell_angle_gamma 90.00
_cell_volume 863.947
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.18824 0.43445 -0.08181
H*2 H 0.12925 0.40127 -0.15130
H*3 H 0.26754 0.37087 -0.09193
H*4 H 0.22615 0.52514 -0.12237
H*5 H 0.13002 0.44051 0.03837
C1+ C 0.18283 -0.09686 0.79434
N'2+ N 0.03170 -0.24867 0.80980
N'3+ N -0.00145 -0.14127 0.74278
N'4+ N 0.08846 -0.04638 0.73171
N5+ N 0.14815 -0.22198 0.84397
C6+ C 0.30215 -0.03449 0.81793
N7+ N 0.44345 -0.07683 0.69344
O8+ O 0.53930 -0.00365 0.68219
O9+ O 0.44362 -0.17762 0.61963
N10+ N 0.29776 0.11453 0.79651
O11+ O 0.30980 0.14972 0.65751
O12+ O 0.28248 0.18352 0.91623
N13+ N 0.31492 -0.06416 0.99360
O14+ O 0.21083 -0.04749 1.10405
O15+ O 0.42547 -0.09714 1.00382
O16+ O 0.21172 -0.29938 0.91202

#END

S14. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylammonium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

data_2b_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 8.740
_cell_length_b 12.546
_cell_length_c 8.556

```
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
_cell_volume                     938.183
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.51401 -0.26026 -0.37219
H*2 H -0.56620 -0.33311 -0.38829
H*3 H -0.57708 -0.21652 -0.29274
H*4 H -0.40414 -0.27266 -0.33160
O5 O -0.51444 -0.21294 -0.52115
H*6 H -0.46564 -0.14325 -0.51101
C1+ C -0.62391 0.55301 0.13130
N'2+ N -0.86184 0.53081 0.19892
N'3+ N -0.81098 0.44532 0.12240
N'4+ N -0.66611 0.45616 0.07900
N5+ N -0.74472 0.60019 0.20502
C6+ C -0.47877 0.60770 0.11194
N7+ N -0.37385 0.61235 0.26306
O8+ O -0.23876 0.63184 0.24127
O9+ O -0.43682 0.59542 0.38675
N10+ N -0.37803 0.55219 -0.01143
O11+ O -0.33128 0.46479 0.02728
O12+ O -0.35413 0.59811 -0.13444
N13+ N -0.50321 0.72762 0.06092
O14+ O -0.59213 0.73942 -0.04635
O15+ O -0.43031 0.79597 0.12863
O16+ O -0.74843 0.69279 0.26647

#END

data_2b_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                   10.191
_cell_length_b                   10.019
_cell_length_c                   8.540
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
```

```
_cell_volume                    871.965
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.85077 -0.14594 0.09174
H*2 H 0.93500 -0.09543 0.06090
H*3 H 0.85618 -0.24214 0.04873
H*4 H 0.84273 -0.14637 0.21231
O5 O 0.74869 -0.07319 0.02117
H*6 H 0.66654 -0.11804 0.04768
C1+ C 0.15150 0.12794 -0.20619
N'2+ N -0.04952 0.05461 -0.20783
N'3+ N -0.02457 0.12242 -0.33876
N'4+ N 0.09727 0.16895 -0.34166
N5+ N 0.06105 0.05763 -0.12198
C6+ C 0.28193 0.15436 -0.14530
N7+ N 0.38120 0.03258 -0.15266
O8+ O 0.49746 0.06014 -0.14174
O9+ O 0.33296 -0.07700 -0.16954
N10+ N 0.35092 0.26557 -0.23888
O11+ O 0.37937 0.23497 -0.37243
O12+ O 0.37059 0.37225 -0.17467
N13+ N 0.27670 0.19716 0.03277
O14+ O 0.19635 0.28278 0.06188
O15+ O 0.35350 0.14481 0.12268
O16+ O 0.07625 0.00579 0.01322

#END

data_2b_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                  8.837
_cell_length_b                  11.879
_cell_length_c                  16.899
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
```

```
_cell_angle_gamma                90.00
_cell_volume                   1773.97
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.22773 0.28808 -0.07965
H*2 H 0.31848 0.24244 -0.05871
H*3 H 0.13491 0.27222 -0.04420
H*4 H 0.25522 0.37258 -0.07869
O5 O 0.20582 0.24866 -0.15725
H*6 H 0.12023 0.29004 -0.17940
C1+ C 0.15721 0.04907 0.60753
N'2+ N -0.08503 0.03181 0.58772
N'3+ N -0.03906 0.13464 0.56728
N'4+ N 0.10830 0.14829 0.57875
N5+ N 0.03805 -0.02350 0.61375
C6+ C 0.30820 0.01764 0.63316
N7+ N 0.39813 -0.06266 0.57473
O8+ O 0.53505 -0.06644 0.58364
O9+ O 0.32313 -0.11259 0.52605
N10+ N 0.41108 0.12167 0.64164
O11+ O 0.44244 0.16751 0.57942
O12+ O 0.45136 0.14959 0.70772
N13+ N 0.30394 -0.04636 0.71515
O14+ O 0.22784 -0.00067 0.76541
O15+ O 0.37799 -0.13208 0.72162
O16+ O 0.04057 -0.12409 0.64011

#END

data_2b_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                 11.803
_cell_length_b                 9.069
_cell_length_c                 9.971
_cell_angle_alpha               90.00
_cell_angle_beta                55.89
_cell_angle_gamma                90.00
_cell_volume                   883.693
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.71691 0.26446 0.66401
H*2 H 0.69072 0.17228 0.62665
H*3 H 0.79222 0.23614 0.68201
H*4 H 0.75141 0.34503 0.57616
O5 O 0.59508 0.30657 0.80935
H*6 H 0.61556 0.39416 0.84908
C1+ C 0.05205 0.34852 0.28453
N'2+ N 0.05233 0.58502 0.32133
N'3+ N -0.07268 0.54007 0.36984
N'4+ N -0.07663 0.39619 0.34884
N5+ N 0.13296 0.46489 0.26612
C6+ C 0.10757 0.20106 0.23190
N7+ N 0.13735 0.11503 0.34753
O8+ O 0.14912 -0.01853 0.33060
O9+ O 0.14488 0.18933 0.44324
N10+ N 0.00752 0.10009 0.22196
O11+ O -0.09649 0.07051 0.35232
O12+ O 0.03863 0.05940 0.08897
N13+ N 0.24829 0.20397 0.06031
O14+ O 0.24684 0.27687 -0.04055
O15+ O 0.34268 0.13216 0.04273
O16+ O 0.26094 0.46246 0.20617

#END

data_2b_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                 7.373
_cell_length_b                 16.972
_cell_length_c                 8.604
_cell_angle_alpha               90.00
_cell_angle_beta                56.01
_cell_angle_gamma                 90.00
_cell_volume                   892.695
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.03969 0.16932 0.31834
H*2 H -0.06755 0.15785 0.45933
H*3 H -0.01134 0.13909 0.24511
H*4 H 0.04207 0.22928 0.29671
O5 O 0.24290 0.14184 0.27498
H*6 H 0.34991 0.15166 0.14169
C1+ C 0.50227 0.63804 0.11306
N'2+ N 0.82656 0.68356 0.01099
N'3+ N 0.78769 0.68862 -0.12249
N'4+ N 0.59121 0.66119 -0.06521
N5+ N 0.64738 0.65124 0.16127
C6+ C 0.29195 0.60094 0.24178
N7+ N 0.11094 0.65606 0.40351
O8+ O -0.07807 0.63387 0.48140
O9+ O 0.17606 0.71561 0.43466
N10+ N 0.18734 0.57214 0.13919
O11+ O 0.12978 0.62463 0.07968
O12+ O 0.17154 0.50146 0.12507
N13+ N 0.31463 0.52835 0.34493
O14+ O 0.46056 0.48309 0.24174
O15+ O 0.18456 0.52289 0.51351
O16+ O 0.62184 0.63528 0.31723

#END
```

S15. Optimized crystal structure coordinates for 5 polymorphs of Hydrazinium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

```
data_2c_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                 11.920
_cell_length_b                 11.833
_cell_length_c                 12.774
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   1801.76
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.21488 0.01495 0.23444
H*2 H 0.27411 -0.03916 0.26473
H*3 H 0.14669 0.01133 0.28367
N4 N 0.18089 -0.02781 0.13307
H*5 H 0.12120 0.02565 0.10406
H*6 H 0.24935 -0.02513 0.08502
H*7 H 0.24676 0.09610 0.23551
C1+ C -0.03923 0.76929 0.05884
N'2+ N -0.14585 0.75705 0.19668
N'3+ N -0.15123 0.86077 0.15631
N'4+ N -0.08695 0.87141 0.07212
N5+ N -0.07470 0.69798 0.13602
C6+ C 0.04190 0.73376 -0.01926
N7+ N -0.00604 0.65567 -0.10973
O8+ O 0.05065 0.64916 -0.18903
O9+ O -0.09508 0.60995 -0.09246
N10+ N 0.09212 0.83591 -0.07757
O11+ O 0.02618 0.88544 -0.13389
O12+ O 0.19049 0.85895 -0.06309
N13+ N 0.14096 0.66429 0.03205
O14+ O 0.18145 0.70800 0.10905
O15+ O 0.16952 0.57677 -0.01001
O16+ O -0.04556 0.59536 0.14996

#END

data_2c_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                 17.498
_cell_length_b                 6.926
_cell_length_c                 7.904
_cell_angle_alpha               90.00
_cell_angle_beta                86.76
_cell_angle_gamma                 90.00
_cell_volume                   956.364
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.42439 -0.06676 0.27939
H*2 H 0.46671 0.01870 0.22329
H*3 H 0.43482 -0.07458 0.40599
N4 N 0.43226 -0.25891 0.20826
H*5 H 0.39060 -0.34334 0.26595
H*6 H 0.42267 -0.24953 0.08221
H*7 H 0.37219 -0.00010 0.26713
C1+ C 0.61074 0.45674 0.23708
N'2+ N 0.56712 0.22047 0.39638
N'3+ N 0.54029 0.20711 0.24230
N'4+ N 0.56563 0.34934 0.14165
N5+ N 0.61169 0.37869 0.39552
C6+ C 0.65130 0.63422 0.19314
N7+ N 0.74115 0.61333 0.15944
O8+ O 0.77335 0.74456 0.08095
O9+ O 0.76985 0.46833 0.21357
N10+ N 0.62404 0.72129 0.02757
O11+ O 0.64119 0.62700 -0.09872
O12+ O 0.58830 0.87224 0.03529
N13+ N 0.63984 0.78992 0.33865
O14+ O 0.57393 0.81220 0.39049
O15+ O 0.69602 0.87553 0.38255
O16+ O 0.64685 0.44310 0.52080

#END

data_2c_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                 8.727
_cell_length_b                 8.764
_cell_length_c                 12.480
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   954.513
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.73196 -0.38873 -0.01474
H*2 H 0.83968 -0.43496 -0.02281
H*3 H 0.68823 -0.37744 -0.09087
N4 N 0.74788 -0.23765 0.03090
H*5 H 0.64062 -0.19189 0.03753
H*6 H 0.79294 -0.24974 0.10598
H*7 H 0.66415 -0.46422 0.02757
C1+ C 0.62502 0.11379 -0.18954
N'2+ N 0.38873 0.03803 -0.20632
N'3+ N 0.42999 0.12112 -0.29100
N'4+ N 0.57357 0.16961 -0.28339
N5+ N 0.51101 0.03279 -0.14086
C6+ C 0.77310 0.13574 -0.13883
N7+ N 0.88507 -0.00670 -0.14306
O8+ O 1.02047 0.01966 -0.12722
O9+ O 0.82651 -0.12898 -0.16237
N10+ N 0.86423 0.26471 -0.19342
O11+ O 0.90642 0.23552 -0.28400
O12+ O 0.88585 0.38238 -0.14376
N13+ N 0.75496 0.17568 -0.01594
O14+ O 0.66213 0.27501 0.00268
O15+ O 0.83575 0.10837 0.04775
O16+ O 0.51670 -0.03385 -0.05009

#END

data_2c_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                 8.725
_cell_length_b                 10.323
_cell_length_c                 10.311
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   928.693
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

N1 N 0.43405 -0.30201 -0.11411
H*2 H 0.33001 -0.30837 -0.16060
H*3 H 0.48449 -0.39180 -0.12130
N4 N 0.40553 -0.27589 0.02174
H*5 H 0.50928 -0.27117 0.06745
H*6 H 0.35391 -0.18727 0.02793
H*7 H 0.50154 -0.23540 -0.16232
C1+ C 0.38045 0.06731 0.12822
N'2+ N 0.16076 0.07620 0.22781
N'3+ N 0.15590 -0.01161 0.13313
N'4+ N 0.28806 -0.01949 0.07002
N5+ N 0.30232 0.12767 0.22569
C6+ C 0.53692 0.10263 0.09595
N7+ N 0.66450 0.04862 0.19129
O8+ O 0.79536 0.04722 0.14957
O9+ O 0.62069 0.01267 0.29682
N10+ N 0.58353 0.04933 -0.03795
O11+ O 0.59500 -0.06798 -0.04265
O12+ O 0.60400 0.12588 -0.12614
N13+ N 0.55862 0.25468 0.09515
O14+ O 0.46137 0.31300 0.03491
O15+ O 0.66970 0.29926 0.15054
O16+ O 0.35162 0.21717 0.30009

#END

data_2c_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 17.586
_cell_length_b 9.779
_cell_length_c 11.494
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1976.66
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x

```
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.62740 0.41419 0.48294
H*2 H 0.67325 0.47776 0.49573
H*3 H 0.59344 0.42339 0.55538
N4 N 0.65509 0.27487 0.47772
H*5 H 0.60916 0.21231 0.46632
H*6 H 0.68942 0.26700 0.40633
H*7 H 0.59739 0.44796 0.41125
C1+ C 0.06776 0.63826 0.28072
N'2+ N -0.05352 0.67335 0.25774
N'3+ N -0.02527 0.60692 0.16617
N'4+ N 0.04873 0.58398 0.17709
N5+ N 0.00485 0.69462 0.33110
C6+ C 0.14207 0.64664 0.33524
N7+ N 0.15575 0.54435 0.44029
O8+ O 0.22187 0.52357 0.46716
O9+ O 0.09939 0.49512 0.48410
N10+ N 0.20594 0.61205 0.24831
O11+ O 0.20721 0.49315 0.21737
O12+ O 0.24866 0.70323 0.21773
N13+ N 0.15721 0.79429 0.38624
O14+ O 0.14306 0.88674 0.31948
O15+ O 0.18281 0.80289 0.48418
O16+ O 0.00133 0.75746 0.42819

#END
```

S16. Optimized crystal structure coordinates for 5 polymorphs of Guanidinium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

```
data_2d_1
_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                 16.357
_cell_length_b                 8.434
_cell_length_c                 7.621
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1051.35
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25871 0.75349 0.54461
N2 N 0.18174 0.76982 0.60098
H*3 H 0.14589 0.67442 0.62371
H*4 H 0.15718 0.87804 0.62249
N5 N 0.28962 0.60879 0.51724
H*6 H 0.34762 0.59377 0.47467
H*7 H 0.25588 0.51023 0.53833
N8 N 0.30477 0.88186 0.51561
H*9 H 0.28262 0.99227 0.53545
H*10 H 0.36306 0.87219 0.47301
C1+ C 0.39632 0.21930 0.26276
N'2+ N 0.29448 0.31038 0.10907
N'3+ N 0.29319 0.15237 0.11084
N'4+ N 0.35463 0.09260 0.20322
N5+ N 0.35979 0.35486 0.20427
C6+ C 0.47086 0.22362 0.36603
N7+ N 0.45955 0.27041 0.56617
O8+ O 0.51561 0.23537 0.66443
O9+ O 0.39603 0.33584 0.60413
N10+ N 0.51230 0.05964 0.37233
O11+ O 0.47461 -0.03995 0.45461
O12+ O 0.57723 0.04238 0.29646
N13+ N 0.53389 0.34758 0.28908
O14+ O 0.54452 0.33722 0.13215
O15+ O 0.56710 0.43787 0.39089
O16+ O 0.38299 0.49717 0.23133

#END

data_2d_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                 9.716
_cell_length_b                 10.107
_cell_length_c                 6.006
_cell_angle_alpha               81.05
_cell_angle_beta                67.56
_cell_angle_gamma                91.34
_cell_volume                   536.274
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.31419 0.27089 -0.17101
N2 N 0.24883 0.27867 0.06641
H*3 H 0.22238 0.36761 0.12136
H*4 H 0.22397 0.19585 0.19780
N5 N 0.34581 0.38216 -0.34097
H*6 H 0.39517 0.37854 -0.52134
H*7 H 0.32126 0.47312 -0.29400
N8 N 0.34794 0.15183 -0.23847
H*9 H 0.32503 0.06652 -0.11305
H*10 H 0.39734 0.14369 -0.41683
C1+ C 0.70305 0.22173 -0.07611
N'2+ N 0.53373 0.30320 0.21366
N'3+ N 0.50347 0.17083 0.24278
N'4+ N 0.60442 0.11769 0.06873
N5+ N 0.65975 0.33731 0.01138
C6+ C 0.83367 0.22249 -0.29954
N7+ N 0.98993 0.23632 -0.27470
O8+ O 1.09664 0.20246 -0.43672
O9+ O 0.98946 0.27841 -0.09625
N10+ N 0.83438 0.09002 -0.39674
O11+ O 0.85334 -0.00775 -0.26910
O12+ O 0.81586 0.09286 -0.58683
N13+ N 0.84054 0.34319 -0.50657
O14+ O 0.72433 0.35457 -0.53552
O15+ O 0.95909 0.41071 -0.62063
O16+ O 0.72392 0.45590 -0.08071

#END

data_2d_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                 8.194
_cell_length_b                 7.398
_cell_length_c                 9.061
_cell_angle_alpha               84.84
_cell_angle_beta                89.98
_cell_angle_gamma                90.57
_cell_volume                   547.017
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

```
_atom_site_fract_z
C1 C 0.55628 -0.26473 0.80803
N2 N 0.65215 -0.27329 0.68943
H*3 H 0.77450 -0.28481 0.69967
H*4 H 0.60504 -0.26847 0.58610
N5 N 0.62197 -0.27141 0.94348
H*6 H 0.55177 -0.26516 1.03458
H*7 H 0.74373 -0.28290 0.95870
N8 N 0.39472 -0.24950 0.79118
H*9 H 0.34257 -0.24422 0.68985
H*10 H 0.32006 -0.24282 0.87929
C1+ C -0.21969 0.23894 0.66677
N'2+ N -0.48264 0.25534 0.69579
N'3+ N -0.44629 0.24791 0.55308
N'4+ N -0.28666 0.23818 0.53116
N5+ N -0.34011 0.25060 0.76950
C6+ C -0.04847 0.23697 0.70794
N7+ N 0.01572 0.04982 0.78442
O8+ O 0.16329 0.02925 0.78460
O9+ O -0.08742 -0.05677 0.83504
N10+ N 0.06233 0.27599 0.57110
O11+ O 0.06221 0.15666 0.48715
O12+ O 0.13849 0.41872 0.55733
N13+ N -0.00962 0.38229 0.82106
O14+ O -0.06330 0.53186 0.78531
O15+ O 0.07184 0.33504 0.92954
O16+ O -0.32280 0.25833 0.90869

#END

data_2d_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                 8.107
_cell_length_b                 9.161
_cell_length_c                 14.166
_cell_angle_alpha               90.00
_cell_angle_beta                93.82
_cell_angle_gamma                 90.00
_cell_volume                   1049.75
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.04546 -0.30516 0.63024
N2 N -0.14055 -0.18576 0.62752
H*3 H -0.26482 -0.19299 0.62843
H*4 H -0.09092 -0.08482 0.62447
N5 N -0.11452 -0.43739 0.63426
H*6 H -0.04496 -0.52902 0.63637
H*7 H -0.23827 -0.44955 0.63530
N8 N 0.11869 -0.29233 0.62894
H*9 H 0.17340 -0.19348 0.62592
H*10 H 0.19282 -0.38111 0.63095
C1+ C 0.29939 0.32844 0.11994
N'2+ N 0.03215 0.31658 0.12575
N'3+ N 0.08020 0.45517 0.11940
N'4+ N 0.24279 0.46660 0.11590
N5+ N 0.16987 0.23466 0.12661
C6+ C 0.46878 0.27656 0.12194
N7+ N 0.52214 0.20527 0.02659
O8+ O 0.67047 0.19619 0.01773
O9+ O 0.41100 0.16700 -0.02936
N10+ N 0.59276 0.40233 0.14091
O11+ O 0.59614 0.49043 0.07686
O12+ O 0.67471 0.40446 0.21615
N13+ N 0.50285 0.15597 0.20066
O14+ O 0.45575 0.18809 0.27736
O15+ O 0.57495 0.04574 0.17926
O16+ O 0.17627 0.09596 0.13373

#END

data_2d_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                 15.961
_cell_length_b                 7.294
_cell_length_c                 9.025
_cell_angle_alpha               90.00
_cell_angle_beta                91.56
_cell_angle_gamma                 90.00
_cell_volume                   1050.3
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.77332 -0.22071 -0.17544
N2 N 0.80721 -0.20171 -0.03915
H*3 H 0.86994 -0.20594 -0.02110
H*4 H 0.77107 -0.18257 0.04975
N5 N 0.82267 -0.24587 -0.29109
H*6 H 0.79837 -0.26054 -0.39498
H*7 H 0.88571 -0.25097 -0.27797
N8 N 0.69008 -0.21454 -0.19608
H*9 H 0.65165 -0.19566 -0.11024
H*10 H 0.66318 -0.22859 -0.29811
C1+ C -0.10185 0.24602 0.65713
N'2+ N -0.23665 0.26288 0.68478
N'3+ N -0.21963 0.23837 0.54238
N'4+ N -0.13785 0.22784 0.52129
N5+ N -0.16255 0.26887 0.75915
C6+ C -0.01343 0.25121 0.69910
N7+ N 0.02230 0.07158 0.77715
O8+ O 0.09826 0.05261 0.77817
O9+ O -0.02899 -0.03163 0.82799
N10+ N 0.04142 0.27546 0.56259
O11+ O 0.04154 0.14420 0.47952
O12+ O 0.07894 0.41948 0.54819
N13+ N 0.00643 0.41289 0.81132
O14+ O -0.02303 0.55952 0.77429
O15+ O 0.05003 0.37925 0.92044
O16+ O -0.15206 0.29393 0.89829

#END
```

S17. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidinium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

```
data_2e_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                 8.011
_cell_length_b                 22.680
_cell_length_c                 6.281
_cell_angle_alpha               90.00
_cell_angle_beta                83.73
_cell_angle_gamma                90.00
```

```
_cell_volume                    1134.37
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.21577 0.32451 0.02376
N2 N 0.15812 0.27195 -0.03258
H*3 H 0.07919 0.26831 -0.14685
H*4 H 0.19210 0.23443 0.03786
N5 N 0.16743 0.37348 -0.07404
H*6 H 0.08818 0.37013 -0.18895
N7 N 0.31962 0.32925 0.17416
H*8 H 0.35865 0.29355 0.25105
H*9 H 0.35949 0.37009 0.21069
N10 N 0.22807 0.42826 -0.01450
H*11 H 0.29531 0.44786 -0.14227
H*12 H 0.13103 0.45469 0.04435
C1+ C 0.17995 0.64311 0.45948
N'2+ N 0.11243 0.73160 0.57195
N'3+ N 0.04731 0.72051 0.38970
N'4+ N 0.08629 0.66687 0.31606
N5+ N 0.19770 0.68301 0.61809
C6+ C 0.26131 0.58586 0.45536
N7+ N 0.17449 0.53851 0.61719
O8+ O 0.21169 0.48710 0.57958
O9+ O 0.07799 0.55749 0.76307
N10+ N 0.26309 0.55640 0.23409
O11+ O 0.12553 0.54148 0.18865
O12+ O 0.39725 0.55068 0.12461
N13+ N 0.44838 0.59112 0.51147
O14+ O 0.52978 0.62942 0.41385
O15+ O 0.49533 0.55648 0.64001
O16+ O 0.28073 0.67651 0.77859

#END

data_2e_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                  11.253
_cell_length_b                  10.291
_cell_length_c                  10.427
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 113.97
_cell_angle_gamma                90.00
_cell_volume                     1103.36
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.40327 0.14854 0.35108
N2 N 0.32856 0.09576 0.40981
H*3 H 0.31198 -0.00095 0.40589
H*4 H 0.28668 0.15138 0.45975
N5 N 0.45733 0.07100 0.28547
H*6 H 0.44106 -0.02622 0.28116
N7 N 0.42504 0.27582 0.35630
H*8 H 0.38620 0.33706 0.40452
H*9 H 0.48234 0.31072 0.31013
N10 N 0.53528 0.12669 0.22432
H*11 H 0.62731 0.09041 0.26960
H*12 H 0.49645 0.10950 0.11904
C1+ C 0.85585 -0.18566 0.25933
N'2+ N 0.77634 -0.20951 0.41647
N'3+ N 0.80966 -0.32457 0.38246
N'4+ N 0.85836 -0.31376 0.28648
N5+ N 0.80447 -0.12026 0.33879
C6+ C 0.89352 -0.11886 0.15898
N7+ N 1.02709 -0.04204 0.22434
O8+ O 1.07726 -0.01462 0.14380
O9+ O 1.06801 -0.01811 0.34865
N10+ N 0.91245 -0.21506 0.05558
O11+ O 1.00556 -0.28691 0.10831
O12+ O 0.83516 -0.21248 -0.06679
N13+ N 0.78813 -0.01490 0.07201
O14+ O 0.67737 -0.05509 0.02398
O15+ O 0.82574 0.09265 0.05780
O16+ O 0.78454 0.00173 0.33910

#END

data_2e_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                 7.222
_cell_length_b                 6.580
_cell_length_c                 32.615
_cell_angle_alpha               90.00
_cell_angle_beta                46.09
_cell_angle_gamma                 90.00
_cell_volume                   1116.59
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.85820 0.08438 0.66586
N2 N 0.62335 0.13050 0.71598
H*3 H 0.46476 0.10823 0.72303
H*4 H 0.59842 0.18896 0.74817
N5 N 0.88318 0.00672 0.62404
H*6 H 0.72465 -0.01602 0.63084
N7 N 1.06678 0.11374 0.65663
H*8 H 1.05579 0.17164 0.68693
H*9 H 1.23991 0.07623 0.61792
N10 N 1.12898 -0.04117 0.57178
H*11 H 1.14110 -0.19235 0.56349
H*12 H 1.17004 0.04233 0.54001
C1+ C 0.26256 -0.12503 0.15577
N'2+ N 0.00476 -0.18169 0.24665
N'3+ N -0.12897 -0.12657 0.23415
N'4+ N 0.02233 -0.09032 0.17901
N5+ N 0.25385 -0.18061 0.19740
C6+ C 0.50484 -0.10198 0.09698
N7+ N 0.63947 -0.30756 0.06275
O8+ O 0.80231 -0.29366 0.01097
O9+ O 0.56761 -0.46051 0.09100
N10+ N 0.46953 0.01620 0.06201
O11+ O 0.34794 -0.07434 0.05460
O12+ O 0.56171 0.18583 0.04521
N13+ N 0.70967 0.01335 0.09274
O14+ O 0.63022 0.16747 0.12084
O15+ O 0.92540 -0.05685 0.06153
O16+ O 0.44373 -0.22133 0.19158

#END

data_2e_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                 8.673
_cell_length_b                10.444
_cell_length_c                12.646
_cell_angle_alpha               90.00
_cell_angle_beta               102.51
_cell_angle_gamma                90.00
_cell_volume                  1118.29
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24796 -0.26040 0.77079
N2 N 0.35510 -0.33792 0.74222
H*3 H 0.41021 -0.31397 0.68236
H*4 H 0.38377 -0.42265 0.77986
N5 N 0.21308 -0.14824 0.71859
H*6 H 0.26801 -0.12361 0.65839
N7 N 0.17550 -0.29201 0.84958
H*8 H 0.19851 -0.37526 0.89056
H*9 H 0.09538 -0.22985 0.86797
N10 N 0.10106 -0.06767 0.74879
H*11 H 0.15120 0.01786 0.77550
H*12 H 0.00817 -0.05388 0.68509
C1+ C -0.37097 0.71289 0.02929
N'2+ N -0.43511 0.55394 0.12243
N'3+ N -0.55385 0.63737 0.09845
N'4+ N -0.51873 0.73588 0.04177
N5+ N -0.31773 0.60069 0.07955
C6+ C -0.27141 0.79154 -0.02311
N7+ N -0.25111 0.74229 -0.13797
O8+ O -0.20460 0.82092 -0.19527
O9+ O -0.28458 0.63121 -0.15903
N10+ N -0.33942 0.92758 -0.04551
O11+ O -0.46178 0.93288 -0.11385
O12+ O -0.26849 1.01645 0.00543
N13+ N -0.09830 0.80228 0.04859
O14+ O -0.09242 0.82878 0.14266
O15+ O 0.01160 0.78672 0.00445
O16+ O -0.18230 0.54961 0.08660

#END

data_2e_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 12.003
_cell_length_b 7.189
_cell_length_c 6.752
_cell_angle_alpha 88.46
_cell_angle_beta 90.63
_cell_angle_gamma 82.09
_cell_volume 576.812
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.82819 -0.06486 0.16625
N2 N 0.92692 -0.01691 0.22595
H*3 H 0.93685 0.11870 0.24559
H*4 H 0.99429 -0.11533 0.25302
N5 N 0.74041 0.07063 0.13174
H*6 H 0.74983 0.20711 0.15118
N7 N 0.81520 -0.24337 0.14045
H*8 H 0.87903 -0.34884 0.16482
H*9 H 0.73869 -0.27194 0.09507
N10 N 0.63749 0.01968 0.06940
H*11 H 0.57671 0.06012 0.16959
H*12 H 0.61512 0.07898 -0.06647
C1+ C 0.18002 0.40472 0.32745
N'2+ N 0.00433 0.47233 0.23615
N'3+ N 0.02821 0.28992 0.28364
N'4+ N 0.13490 0.24347 0.33973
N5+ N 0.09992 0.54723 0.26226
C6+ C 0.29536 0.43522 0.36486
N7+ N 0.31656 0.53543 0.56560
O8+ O 0.41379 0.51884 0.62552
O9+ O 0.23428 0.61856 0.64252
N10+ N 0.37498 0.24787 0.38051
O11+ O 0.36096 0.15089 0.52603
O12+ O 0.44325 0.21171 0.25015
N13+ N 0.33855 0.56215 0.19529
O14+ O 0.31997 0.51407 0.02888
O15+ O 0.38785 0.69089 0.24388
O16+ O 0.11233 0.71861 0.22899

#END

S18. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidinium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

data_2f_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                 18.469
_cell_length_b                 10.272
_cell_length_c                 6.400
_cell_angle_alpha               90.00
_cell_angle_beta                95.78
_cell_angle_gamma               90.00
_cell_volume                   1207.99
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.42499 -0.37961 0.39266
N2 N 0.44999 -0.27955 0.51311
H*3 H 0.42011 -0.25099 0.63002
N4 N 0.36216 -0.43746 0.43088
H*5 H 0.34279 -0.51334 0.34046
N6 N 0.46188 -0.42127 0.23706
H*7 H 0.50887 -0.37484 0.21404
H*8 H 0.44427 -0.49646 0.14391
N9 N 0.32482 -0.39115 0.59568
N10 N 0.51535 -0.21979 0.47262
H*11 H 0.55247 -0.22738 0.60095
H*12 H 0.27443 -0.35902 0.53964
H*13 H 0.32068 -0.46244 0.70436
H*14 H 0.50632 -0.12421 0.43661
C1+ C 0.13127 0.67316 0.02296
N'2+ N 0.13191 0.86410 0.17052
N'3+ N 0.09421 0.86792 -0.01826
N'4+ N 0.09280 0.75302 -0.11319
N5+ N 0.15612 0.74128 0.19884
C6+ C 0.14947 0.53696 -0.00235
N7+ N 0.10539 0.43706 0.12520
O8+ O 0.10522 0.32406 0.06638
O9+ O 0.07535 0.48184 0.26889
N10+ N 0.13349 0.49318 -0.23266
O11+ O 0.06917 0.48966 -0.29577
O12+ O 0.18464 0.46686 -0.33117
N13+ N 0.23247 0.51018 0.07057
O14+ O 0.27413 0.58607 0.00080
O15+ O 0.24749 0.41666 0.18298
```

```
O16+ O 0.19561 0.69863 0.35924

#END

data_2f_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                 12.207
_cell_length_b                 11.885
_cell_length_c                 11.012
_cell_angle_alpha               90.00
_cell_angle_beta                50.92
_cell_angle_gamma                 90.00
_cell_volume                   1240.18
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.26117 0.23457 0.04876
N2 N -0.36597 0.29268 0.17410
H*3 H -0.41546 0.35211 0.15774
N4 N -0.22619 0.25697 -0.09184
H*5 H -0.14694 0.21338 -0.18747
N6 N -0.19252 0.15564 0.06320
H*7 H -0.22242 0.14164 0.17119
H*8 H -0.11315 0.11060 -0.02933
N9 N -0.30056 0.34047 -0.10272
N10 N -0.40187 0.26902 0.31998
H*11 H -0.50413 0.24302 0.39610
H*12 H -0.23396 0.40314 -0.17551
H*13 H -0.34984 0.30687 -0.14200
H*14 H -0.38853 0.33907 0.36267
C1+ C 0.18257 0.02032 0.52047
N'2+ N 0.02147 0.06133 0.76678
N'3+ N -0.00473 0.11436 0.68084
N'4+ N 0.09173 0.09146 0.52970
N5+ N 0.14039 0.00162 0.66673
C6+ C 0.31119 -0.02888 0.38253
N7+ N 0.30137 -0.15809 0.35433
O8+ O 0.39250 -0.19346 0.22231
O9+ O 0.20373 -0.21014 0.46603
N10+ N 0.35680 0.02933 0.23195
```

O11+ O 0.27850 0.01258 0.20106
O12+ O 0.46372 0.08620 0.15807
N13+ N 0.43634 -0.02009 0.38956
O14+ O 0.45105 0.07243 0.42372
O15+ O 0.50772 -0.10346 0.35736
O16+ O 0.20181 -0.05919 0.70328

#END

data_2f_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 10.774
_cell_length_b 6.507
_cell_length_c 9.629
_cell_angle_alpha 81.56
_cell_angle_beta 67.62
_cell_angle_gamma 85.56
_cell_volume 617.278
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.35580 -0.09564 -0.34799
N2 N 0.25781 0.02394 -0.37326
H*3 H 0.21807 0.14008 -0.30802
N4 N 0.39707 -0.05760 -0.23868
H*5 H 0.47125 -0.14736 -0.21870
N6 N 0.41164 -0.25022 -0.43004
H*7 H 0.37742 -0.27314 -0.51104
H*8 H 0.48565 -0.34270 -0.41336
N9 N 0.33617 0.10612 -0.15463
N10 N 0.21532 -0.01637 -0.48706
H*11 H 0.23024 0.11029 -0.56696
H*12 H 0.29105 0.05127 -0.04293
H*13 H 0.40540 0.21332 -0.16884
H*14 H 0.11616 -0.05138 -0.44134
C1+ C -0.25124 0.47556 0.75855
N'2+ N -0.42404 0.34570 0.74087
N'3+ N -0.39976 0.53433 0.66202
N'4+ N -0.29502 0.61860 0.67050
N5+ N -0.33104 0.30630 0.80348
C6+ C -0.14201 0.48830 0.80995
N7+ N -0.01040 0.35690 0.72892

```
O8+ O 0.09229 0.40564 0.73986
O9+ O -0.02318 0.22065 0.66242
N10+ N -0.09318 0.71272 0.78082
O11+ O -0.03707 0.77840 0.64778
O12+ O -0.11421 0.80472 0.88931
N13+ N -0.18585 0.40938 0.98479
O14+ O -0.29215 0.48197 1.06333
O15+ O -0.11025 0.29001 1.02556
O16+ O -0.32178 0.14235 0.88993

#END

data_2f_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                 7.653
_cell_length_b                 8.461
_cell_length_c                 9.849
_cell_angle_alpha               101.31
_cell_angle_beta                86.14
_cell_angle_gamma                76.62
_cell_volume                   604.123
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.03614 0.26200 0.81461
N2 N -0.05317 0.22203 0.67858
H*3 H 0.05278 0.21974 0.60955
N4 N 0.11852 0.29704 0.85376
H*5 H 0.13267 0.32745 0.95658
N6 N -0.17065 0.26699 0.90985
H*7 H -0.28450 0.23972 0.87563
H*8 H -0.16139 0.29674 1.01303
N9 N 0.25707 0.29059 0.75088
N10 N -0.21431 0.18573 0.63851
H*11 H -0.18781 0.06734 0.58046
H*12 H 0.28418 0.40422 0.75995
H*13 H 0.37060 0.20363 0.75851
H*14 H -0.27404 0.26746 0.58191
C1+ C 0.19755 0.27524 0.23476
N'2+ N -0.07178 0.25396 0.30035
N'3+ N -0.07485 0.32400 0.19026
N'4+ N 0.08732 0.33930 0.14751
```

N5+ N 0.10001 0.22287 0.33040
C6+ C 0.38896 0.26506 0.23935
N7+ N 0.51984 0.08529 0.18238
O8+ O 0.67840 0.07998 0.15102
O9+ O 0.45070 -0.03087 0.17410
N10+ N 0.45515 0.37354 0.14858
O11+ O 0.45612 0.32398 0.02391
O12+ O 0.49923 0.49690 0.20641
N13+ N 0.43143 0.32266 0.39356
O14+ O 0.33193 0.45315 0.45738
O15+ O 0.55921 0.23631 0.43336
O16+ O 0.15797 0.15877 0.43081

#END

data_2f_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 7.220
_cell_length_b 10.129
_cell_length_c 18.178
_cell_angle_alpha 90.00
_cell_angle_beta 78.51
_cell_angle_gamma 90.00
_cell_volume 1302.74
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.52993 0.30219 0.63892
N2 N 0.41676 0.39459 0.67673
H*3 H 0.29952 0.42029 0.65701
N4 N 0.48435 0.24790 0.57719
H*5 H 0.56923 0.17783 0.54818
N6 N 0.68557 0.26458 0.66215
H*7 H 0.71427 0.30809 0.70886
H*8 H 0.77333 0.19517 0.63472
N9 N 0.31974 0.28978 0.55439
N10 N 0.46488 0.45068 0.74086
H*11 H 0.36062 0.43291 0.78644
H*12 H 0.35218 0.32989 0.50204
H*13 H 0.22891 0.21271 0.55506

H*14 H 0.48360 0.54982 0.73355
C1+ C 1.00888 0.35459 -0.10985
N'2+ N 0.90809 0.55303 -0.07806
N'3+ N 1.08926 0.55633 -0.11239
N'4+ N 1.15570 0.43680 -0.13247
N5+ N 0.85501 0.42561 -0.07566
C6+ C 1.00307 0.21169 -0.11506
N7+ N 0.89851 0.15532 -0.17729
O8+ O 0.93338 0.04099 -0.19623
O9+ O 0.79420 0.23097 -0.20092
N10+ N 1.20350 0.15281 -0.13567
O11+ O 1.28698 0.17811 -0.19902
O12+ O 1.26170 0.08813 -0.08854
N13+ N 0.89826 0.14821 -0.03859
O14+ O 0.95049 0.18955 0.01644
O15+ O 0.78076 0.06335 -0.04120
O16+ O 0.69205 0.38107 -0.04590

#END

S19. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidinium 5-(trinitromethyl)tetrazolate 1*N*-oxide (ionic form).

data_2g_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 22.992
_cell_length_b 7.338
_cell_length_c 17.863
_cell_angle_alpha 90.00
_cell_angle_beta 123.12
_cell_angle_gamma 90.00
_cell_volume 2524.11
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.41164 0.64966 0.68288

N2 N 0.40052 0.75959 0.73380
H*3 H 0.39271 0.70020 0.77902
N4 N 0.42223 0.72098 0.62218
H*5 H 0.42144 0.85900 0.61683
N6 N 0.41216 0.46841 0.69266
H*7 H 0.42077 0.38978 0.65279
N8 N 0.43373 0.60315 0.56979
N9 N 0.40023 0.94856 0.72227
H*10 H 0.43825 1.00787 0.78027
H*11 H 0.39619 0.62125 0.50393
H*12 H 0.48123 0.62804 0.58029
H*13 H 0.35321 1.00109 0.70390
N14 N 0.40096 0.39727 0.75657
H*15 H 0.35796 0.31646 0.72626
H*16 H 0.44300 0.32325 0.80263
C1+ C 0.10433 0.34337 0.51027
N'2+ N -0.00657 0.29231 0.44288
N'3+ N 0.00743 0.36660 0.38633
N'4+ N 0.07468 0.40002 0.42525
N5+ N 0.05435 0.27734 0.52201
C6+ C 0.17667 0.35305 0.58369
N7+ N 0.21764 0.16556 0.61081
O8+ O 0.28087 0.17599 0.65458
O9+ O 0.18256 0.02852 0.58517
N10+ N 0.21864 0.47825 0.56078
O11+ O 0.22595 0.41945 0.50277
O12+ O 0.24033 0.62207 0.60076
N13+ N 0.18410 0.42642 0.67174
O14+ O 0.15067 0.56271 0.66122
O15+ O 0.22286 0.34546 0.74116
O16+ O 0.06276 0.21536 0.59402

#END

data_2g_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 12.404
_cell_length_b 10.902
_cell_length_c 10.061
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1360.53

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.36666 0.08795 0.61449
N2 N 0.36047 0.18019 0.52670
H*3 H 0.28748 0.22088 0.51370
N4 N 0.46100 0.03114 0.63541
H*5 H 0.52593 0.06074 0.58275
N6 N 0.27851 0.05251 0.68135
H*7 H 0.28657 -0.01776 0.74701
N8 N 0.46535 -0.06501 0.72769
N9 N 0.45375 0.21549 0.45809
H*10 H 0.47145 0.30474 0.47852
H*11 H 0.48918 -0.14372 0.68177
H*12 H 0.51810 -0.04391 0.80182
H*13 H 0.44254 0.20493 0.35847
N14 N 0.18087 0.11337 0.65769
H*15 H 0.12489 0.05292 0.62316
H*16 H 0.15380 0.15273 0.74321
C1+ C 0.13595 0.35292 -0.05245
N'2+ N -0.00732 0.44298 -0.13038
N'3+ N 0.01107 0.33876 -0.19584
N'4+ N 0.09811 0.28140 -0.15107
N5+ N 0.07150 0.45367 -0.03935
C6+ C 0.23182 0.33669 0.02842
N7+ N 0.21093 0.29313 0.17663
O8+ O 0.28786 0.24854 0.23477
O9+ O 0.12028 0.30716 0.21880
N10+ N 0.30631 0.23718 -0.02984
O11+ O 0.27000 0.13370 -0.02408
O12+ O 0.39272 0.26849 -0.07623
N13+ N 0.29784 0.46024 0.04037
O14+ O 0.31317 0.51204 -0.06450
O15+ O 0.32926 0.49085 0.14988
O16+ O 0.08346 0.54257 0.04175

#END

data_2g_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                 12.918
_cell_length_b                 11.358
_cell_length_c                 8.750
_cell_angle_alpha               90.00
_cell_angle_beta                87.99
_cell_angle_gamma                 90.00
_cell_volume                   1283.03
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.78331 0.13891 0.10532
N2 N 0.70556 0.21429 0.08217
H*3 H 0.72226 0.30175 0.08273
N4 N 0.76548 0.02263 0.10569
H*5 H 0.69197 -0.00482 0.08801
N6 N 0.87889 0.17980 0.12810
H*7 H 0.93571 0.11980 0.14522
N8 N 0.84806 -0.05432 0.13015
N9 N 0.60636 0.16933 0.05864
H*10 H 0.58211 0.19459 -0.04589
H*11 H 0.83277 -0.10356 0.22555
H*12 H 0.85913 -0.10826 0.03805
H*13 H 0.55575 0.19929 0.14162
N14 N 0.89551 0.30172 0.12717
H*15 H 0.92187 0.32805 0.23004
H*16 H 0.94823 0.32335 0.04254
C1+ C 0.21470 0.39881 -0.16245
N'2+ N 0.05343 0.35894 -0.10337
N'3+ N 0.06273 0.39748 -0.24707
N'4+ N 0.16019 0.42293 -0.28700
N5+ N 0.14914 0.35973 -0.04768
C6+ C 0.32467 0.41420 -0.13982
N7+ N 0.39113 0.29675 -0.14138
O8+ O 0.48441 0.30830 -0.16287
O9+ O 0.34339 0.20583 -0.12216
N10+ N 0.37571 0.48979 -0.26780
O11+ O 0.37980 0.44282 -0.39276
O12+ O 0.40665 0.58768 -0.23561
N13+ N 0.34466 0.47472 0.01915
O14+ O 0.29255 0.56162 0.04507
O15+ O 0.41044 0.43229 0.09844
O16+ O 0.17261 0.33081 0.08763

#END

data_2g_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                 12.413
_cell_length_b                 6.136
_cell_length_c                 8.870
_cell_angle_alpha               75.36
_cell_angle_beta                84.37
_cell_angle_gamma               91.30
_cell_volume                   649.715
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74038 -0.04861 0.77237
N2 N 0.81546 -0.16992 0.71634
H*3 H 0.79594 -0.24330 0.63129
N4 N 0.76197 0.05171 0.88464
H*5 H 0.83618 0.03173 0.92415
N6 N 0.64372 -0.02762 0.71612
H*7 H 0.58902 0.06575 0.76167
N8 N 0.68213 0.17757 0.94123
N9 N 0.91585 -0.18928 0.77708
H*10 H 0.97639 -0.12437 0.68999
H*11 H 0.66181 0.11075 1.05820
H*12 H 0.71003 0.34073 0.92171
H*13 H 0.92817 -0.35435 0.82648
N14 N 0.62316 -0.13412 0.59880
H*15 H 0.55883 -0.24720 0.63716
H*16 H 0.60705 -0.01722 0.50067
C1+ C -0.30375 0.64966 0.27837
N'2+ N -0.47371 0.53730 0.30493
N'3+ N -0.46351 0.76170 0.25897
N'4+ N -0.36077 0.83635 0.24186
N5+ N -0.37307 0.46342 0.31851
C6+ C -0.18780 0.63163 0.28493
N7+ N -0.12430 0.55420 0.14476
O8+ O -0.02644 0.59380 0.12465
O9+ O -0.17860 0.46395 0.06932
N10+ N -0.13193 0.86093 0.27895
O11+ O -0.13132 1.00043 0.15405
O12+ O -0.09432 0.88491 0.39582
N13+ N -0.16222 0.45526 0.43932
O14+ O -0.21202 0.47844 0.55831
O15+ O -0.09481 0.31842 0.42714
O16+ O -0.34863 0.25792 0.36283

#END
```

```
data_2g_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                 8.257
_cell_length_b                 9.721
_cell_length_c                 16.075
_cell_angle_alpha               90.00
_cell_angle_beta                96.90
_cell_angle_gamma                 90.00
_cell_volume                   1280.94
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.29291 -0.05422 0.50088
N2 N 0.26712 -0.01631 0.42019
H*3 H 0.22326 0.08001 0.40721
N4 N 0.35065 -0.18014 0.52144
H*5 H 0.37332 -0.24380 0.47402
N6 N 0.26096 0.03379 0.56101
H*7 H 0.28215 0.00113 0.62141
N8 N 0.37656 -0.21728 0.60623
N9 N 0.30148 -0.11020 0.35853
H*10 H 0.38818 -0.07076 0.32527
H*11 H 0.30645 -0.30024 0.61667
H*12 H 0.49641 -0.24038 0.62278
H*13 H 0.19822 -0.13062 0.31917
N14 N 0.20068 0.16481 0.53789
H*15 H 0.08912 0.17841 0.55764
H*16 H 0.27908 0.23827 0.56375
C1+ C 0.63136 0.03858 0.14541
N'2+ N 0.38899 0.05323 0.18501
N'3+ N 0.39238 0.11650 0.11168
N'4+ N 0.53865 0.10986 0.08563
N5+ N 0.53995 0.00369 0.20753
C6+ C 0.80352 0.00468 0.15077
N7+ N 0.84337 -0.15078 0.13119
O8+ O 0.98056 -0.17399 0.11376
O9+ O 0.73380 -0.23267 0.13470
N10+ N 0.88876 0.08771 0.08692
O11+ O 0.84704 0.05702 0.01416
```

O12+ O 0.98750 0.17523 0.11310
N13+ N 0.89366 0.03388 0.24147
O14+ O 0.86486 0.14578 0.26947
O15+ O 0.98489 -0.05407 0.27398
O16+ O 0.58726 -0.06154 0.27492

#END

S20. Optimized crystal structure coordinates for 5 polymorphs of Ammonium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

data_3a_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 6.127
_cell_length_b 13.165
_cell_length_c 5.713
_cell_angle_alpha 90.00
_cell_angle_beta 67.05
_cell_angle_gamma 90.00
_cell_volume 424.346
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.24124 -0.20226 -0.07503
H*2 H 0.38789 -0.23870 -0.07049
H*3 H 0.09677 -0.21812 0.08872
H*4 H 0.27070 -0.12522 -0.08880
H*5 H 0.20959 -0.22700 -0.22955
C1+ C -0.24335 0.57285 0.14362
N'2+ N -0.34327 0.50519 0.03652
C3+ C -0.10932 0.54659 0.29364
C4+ C 0.12748 0.49331 0.57380
N'5+ N -0.44904 0.55955 -0.08319
N'6+ N -0.42371 0.65897 -0.05719
N7+ N -0.29378 0.66947 0.08515
N'8+ N 0.01279 0.62062 0.35439
N9+ N 0.13018 0.59126 0.49535
N10+ N 0.00684 0.42251 0.49643
N'11+ N -0.11592 0.44695 0.35850
O12+ O -0.23848 0.75499 0.14936
O13+ O 0.01554 0.33114 0.56266
O14+ O 0.25206 0.65464 0.56006

```
N15+ N 0.24067 0.46675 0.72768
H*16+ H 0.27242 0.39127 0.72914
H*17+ H 0.36465 0.51757 0.72825

#END

data_3a_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                 9.935
_cell_length_b                 13.316
_cell_length_c                 12.329
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1631.06
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.07766 0.40846 0.83381
H*2 H -0.01030 0.43715 0.86488
H*3 H 0.08539 0.33377 0.85390
H*4 H 0.07744 0.41591 0.75083
H*5 H 0.15812 0.44702 0.86563
C1+ C -0.04443 0.86264 0.11993
N'2+ N -0.14695 0.79570 0.11579
C3+ C 0.09645 0.83684 0.12062
C4+ C 0.35259 0.78427 0.12536
N'5+ N -0.25886 0.84929 0.11677
N'6+ N -0.23365 0.94751 0.12209
N7+ N -0.09865 0.95802 0.12395
N'8+ N 0.18825 0.91092 0.10714
N9+ N 0.31623 0.88193 0.10986
N10+ N 0.25360 0.71359 0.13434
N'11+ N 0.12432 0.73761 0.13359
O12+ O -0.03968 1.04247 0.13018
O13+ O 0.29000 0.62273 0.14395
```

O14+ O 0.40983 0.94544 0.09687
N15+ N 0.48458 0.75782 0.13269
H*16+ H 0.50186 0.68373 0.12025
H*17+ H 0.54865 0.80972 0.10193

#END

data_3a_3
_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 6.641
_cell_length_b 9.842
_cell_length_c 14.176
_cell_angle_alpha 90.00
_cell_angle_beta 69.38
_cell_angle_gamma 90.00
_cell_volume 867.195
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.12639 -0.41633 0.58091
H*2 H -0.26919 -0.40690 0.56851
H*3 H -0.02385 -0.33955 0.54415
H*4 H -0.15494 -0.41024 0.65691
H*5 H -0.05757 -0.50863 0.55408
C1+ C -0.29372 0.45260 0.35206
N'2+ N -0.24246 0.34843 0.28535
C3+ C -0.26291 0.59443 0.32559
C4+ C -0.19539 0.85212 0.27210
N'5+ N -0.29516 0.23614 0.33958
N'6+ N -0.37653 0.26265 0.43805
N7+ N -0.37781 0.39895 0.44801
N'8+ N -0.35267 0.68836 0.39798
N9+ N -0.31576 0.81708 0.36856
N10+ N -0.11711 0.75110 0.20276
N'11+ N -0.14591 0.62095 0.22739
O12+ O -0.44339 0.45933 0.53262
O13+ O -0.01360 0.78643 0.11259
O14+ O -0.39470 0.91269 0.43043
N15+ N -0.15247 0.98478 0.24560
H*16+ H -0.10472 1.00165 0.17040

```
H*17+ H -0.25340 1.05095 0.29450

#END

data_3a_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                 9.874
_cell_length_b                 12.920
_cell_length_c                 7.394
_cell_angle_alpha               90.00
_cell_angle_beta                116.68
_cell_angle_gamma                90.00
_cell_volume                   842.836
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.29786 -0.02434 -0.36378
H*2 H 0.21140 -0.06343 -0.35228
H*3 H 0.34785 0.02580 -0.24387
H*4 H 0.37715 -0.07642 -0.36195
H*5 H 0.25504 0.01670 -0.49702
C1+ C -0.33121 0.72234 -0.35794
N'2+ N -0.43503 0.65255 -0.36238
C3+ C -0.18595 0.69676 -0.34796
C4+ C 0.08049 0.64460 -0.32272
N'5+ N -0.55107 0.70700 -0.37116
N'6+ N -0.52685 0.80852 -0.37119
N7+ N -0.38860 0.82034 -0.36332
N'8+ N -0.10382 0.77289 -0.37757
N9+ N 0.02965 0.74404 -0.36399
N10+ N -0.01179 0.57168 -0.30218
N'11+ N -0.14518 0.59551 -0.31158
O12+ O -0.32878 0.90796 -0.35873
O13+ O 0.03528 0.47893 -0.27262
O14+ O 0.11440 0.80934 -0.39143
N15+ N 0.22064 0.61865 -0.30067
H*16+ H 0.23439 0.54186 -0.31486
H*17+ H 0.26532 0.67086 -0.36112

#END
```

```
data_3a_5
_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                 9.851
_cell_length_b                 6.632
_cell_length_c                 13.349
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   872.115
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.33710 0.38811 0.20000
H*2 H 0.34438 0.42034 0.12488
H*3 H 0.34195 0.23469 0.21032
H*4 H 0.41578 0.45604 0.23765
H*5 H 0.24629 0.44137 0.22715
C1+ C 0.20432 -0.00826 0.43196
N'2+ N 0.10188 -0.04215 0.49751
C3+ C 0.34625 -0.00058 0.45786
C4+ C 0.60407 0.01834 0.51097
N'5+ N -0.01119 -0.03708 0.44436
N'6+ N 0.01312 -0.00020 0.34784
N7+ N 0.14880 0.01826 0.33793
N'8+ N 0.43919 0.00171 0.38318
N9+ N 0.56800 0.01112 0.41245
N10+ N 0.50421 0.00797 0.58175
N'11+ N 0.37397 0.00081 0.55762
O12+ O 0.20712 0.05644 0.25520
O13+ O 0.54071 0.00607 0.67285
O14+ O 0.66279 0.01181 0.34829
N15+ N 0.73654 0.03727 0.53827
H*16+ H 0.75538 -0.00276 0.61018
H*17+ H 0.80304 -0.00040 0.48347

#END
```

S21. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylammonium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

```
data_3b_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                 19.339
_cell_length_b                 14.758
_cell_length_c                 5.312
_cell_angle_alpha               90.00
_cell_angle_beta               142.95
_cell_angle_gamma                90.00
_cell_volume                   913.451
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.31631 0.04899 0.20803
H*2 H 0.34653 0.09757 0.17323
H*3 H 0.27379 0.08075 0.23054
H*4 H 0.26170 0.00615 -0.04707
O5 O 0.41521 0.00360 0.57951
H*6 H 0.39021 -0.04333 0.62431
C1+ C -0.16634 -0.30807 0.68870
N'2+ N -0.17074 -0.39950 0.69576
C3+ C -0.10432 -0.25908 0.67766
C4+ C 0.01426 -0.17352 0.67178
N'5+ N -0.23562 -0.41687 0.70540
N'6+ N -0.27268 -0.34115 0.70786
N7+ N -0.23024 -0.27128 0.69657
N'8+ N -0.12214 -0.16881 0.60312
N9+ N -0.06119 -0.12781 0.60195
N10+ N 0.02407 -0.26514 0.72940
N'11+ N -0.03311 -0.30988 0.73906
O12+ O -0.24792 -0.18871 0.70037
O13+ O 0.09108 -0.30669 0.77556
O14+ O -0.07257 -0.04354 0.53067
N15+ N 0.07918 -0.12880 0.68749
H*16+ H 0.11243 -0.16938 0.64865
H*17+ H 0.04859 -0.06664 0.55329

#END

data_3b_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                   7.531
_cell_length_b                   8.379
_cell_length_c                   10.616
_cell_angle_alpha                 110.26
_cell_angle_beta                  89.79
_cell_angle_gamma                    47.80
_cell_volume                     437.827
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.14840 0.17599 -0.23153
H*2 H -0.18645 0.32992 -0.17840
H*3 H 0.03414 0.02627 -0.24119
H*4 H -0.28058 0.19781 -0.17434
O5 O -0.17158 0.16293 -0.36521
H*6 H -0.13675 0.01854 -0.41931
C1+ C -0.21097 0.68263 0.94152
N'2+ N -0.33248 0.62214 0.96141
C3+ C -0.04212 0.58021 0.80648
C4+ C 0.27180 0.37923 0.55669
N'5+ N -0.46689 0.75542 1.09896
N'6+ N -0.43676 0.89775 1.16903
N7+ N -0.27606 0.85557 1.07178
N'8+ N 0.03368 0.68469 0.79720
N9+ N 0.19144 0.57924 0.67002
N10+ N 0.17896 0.29044 0.57364
N'11+ N 0.02378 0.38517 0.69785
O12+ O -0.20339 0.95973 1.10282
O13+ O 0.24788 0.11087 0.46499
O14+ O 0.27125 0.66483 0.64989
N15+ N 0.44253 0.26900 0.42978
H*16+ H 0.44680 0.15974 0.34601
H*17+ H 0.45605 0.37592 0.41821

#END

data_3b_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                19.060
_cell_length_b                14.215
_cell_length_c                5.388
_cell_angle_alpha              90.00
_cell_angle_beta               143.36
_cell_angle_gamma               90.00
_cell_volume                  871.195
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.17159 0.55978 0.34177
H*2 H -0.19674 0.50147 0.16984
H*3 H -0.10187 0.54166 0.65285
H*4 H -0.14777 0.61255 0.28755
O5 O -0.27181 0.58418 0.19576
H*6 H -0.25159 0.63952 0.35174
C1+ C -0.14755 0.30650 0.79645
N'2+ N -0.23048 0.26565 0.70570
C3+ C -0.08486 0.26013 0.77672
C4+ C 0.02958 0.17008 0.74765
N'5+ N -0.26576 0.33126 0.76242
N'6+ N -0.20911 0.41228 0.88810
N7+ N -0.13393 0.39858 0.91134
N'8+ N -0.01855 0.31284 0.80946
N9+ N 0.03782 0.26538 0.79333
N10+ N -0.04263 0.12253 0.70161
N'11+ N -0.10011 0.16541 0.71968
O12+ O -0.06472 0.46166 1.02693
O13+ O -0.05279 0.03448 0.64142
O14+ O 0.10121 0.30839 0.81665
N15+ N 0.09270 0.12320 0.75151
H*16+ H 0.06195 0.05782 0.62681
H*17+ H 0.12213 0.16475 0.69546

#END

data_3b_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                 5.895
_cell_length_b                 14.181
_cell_length_c                 11.671
_cell_angle_alpha               90.00
_cell_angle_beta                110.15
_cell_angle_gamma                 90.00
_cell_volume                   915.944
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.22326 0.41495 0.62477
H*2 H 0.35873 0.46316 0.66387
H*3 H 0.21343 0.40271 0.53594
H*4 H 0.26192 0.35343 0.67519
O5 O 0.01249 0.45837 0.62982
H*6 H -0.12117 0.41472 0.59342
C1+ C 0.37130 0.32155 0.26494
N'2+ N 0.24690 0.24230 0.27010
C3+ C 0.52339 0.33270 0.19208
C4+ C 0.80559 0.34733 0.05967
N'5+ N 0.13161 0.26088 0.34656
N'6+ N 0.17678 0.34799 0.39167
N7+ N 0.32765 0.38799 0.34128
N'8+ N 0.60554 0.41994 0.17992
N9+ N 0.74693 0.42487 0.11264
N10+ N 0.70794 0.26241 0.07276
N'11+ N 0.56820 0.25250 0.13971
O12+ O 0.40993 0.47121 0.36562
O13+ O 0.75678 0.19210 0.01821
O14+ O 0.83101 0.50352 0.09463
N15+ N 0.95973 0.35415 -0.00397
H*16+ H 0.95015 0.29910 -0.06078
H*17+ H 0.97925 0.42067 -0.03090

#END

data_3b_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                 11.332
_cell_length_b                 16.273
_cell_length_c                 5.083
_cell_angle_alpha               90.00
_cell_angle_beta                70.65
_cell_angle_gamma                 90.00
_cell_volume                   884.386
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.67995 0.08519 -0.27472
H*2 H 0.67034 0.03130 -0.37226
H*3 H 0.59298 0.10330 -0.14361
H*4 H 0.74022 0.07516 -0.16370
O5 O 0.72963 0.14146 -0.49344
H*6 H 0.74026 0.19371 -0.40943
C1+ C 0.85677 0.32065 -0.29719
N'2+ N 0.78349 0.30003 -0.45016
C3+ C 0.91181 0.26310 -0.15603
C4+ C 1.00630 0.15460 0.10524
N'5+ N 0.75249 0.36988 -0.54260
N'6+ N 0.80144 0.43460 -0.45525
N7+ N 0.86810 0.40513 -0.29995
N'8+ N 0.99910 0.29061 -0.04888
N9+ N 1.04483 0.23444 0.08107
N10+ N 0.92115 0.13123 -0.01766
N'11+ N 0.87089 0.18428 -0.14726
O12+ O 0.92633 0.45062 -0.18094
O13+ O 0.89090 0.05590 -0.00270
O14+ O 1.12802 0.25382 0.18598
N15+ N 1.05080 0.09951 0.25068
H*16+ H 1.03873 0.04007 0.20598
H*17+ H 1.13125 0.11735 0.27979

#END
```

S22. Optimized crystal structure coordinates for 5 polymorphs of Hydrazinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

```
data_3c_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 6.041
_cell_length_b 14.703
_cell_length_c 11.497
_cell_angle_alpha 90.00
_cell_angle_beta 109.49
_cell_angle_gamma 90.00
_cell_volume 962.66
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.23446 0.08799 0.11729
H*2 H 0.20466 0.09499 0.02428
H*3 H 0.37048 0.04249 0.15000
N4 N 0.02693 0.04820 0.13293
H*5 H 0.05892 0.04054 0.22543
H*6 H -0.10786 0.09335 0.09899
H*7 H 0.28670 0.15006 0.15960
C1+ C 0.38654 0.31829 0.25765
N'2+ N 0.26190 0.24203 0.25942
C3+ C 0.53982 0.32995 0.18590
C4+ C 0.82387 0.34570 0.05536
N'5+ N 0.14543 0.25890 0.33601
N'6+ N 0.18999 0.34206 0.38443
N7+ N 0.34176 0.38117 0.33616
N'8+ N 0.62364 0.41411 0.17703
N9+ N 0.76595 0.41970 0.11061
N10+ N 0.72488 0.26379 0.06512
N'11+ N 0.58406 0.25340 0.13107
O12+ O 0.42369 0.46085 0.36386
O13+ O 0.77348 0.19681 0.00845
O14+ O 0.85171 0.49567 0.09560
N15+ N 0.97854 0.35303 -0.00724
H*16+ H 0.97045 0.30091 -0.06616
H*17+ H 1.00111 0.41758 -0.03208

#END

data_3c_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 9.765
_cell_length_b 6.528
_cell_length_c 14.513
_cell_angle_alpha 90.00
_cell_angle_beta 95.67
_cell_angle_gamma 90.00
_cell_volume 920.618
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.20643 0.12471 0.51481
H*2 H -0.15834 0.08775 0.45709
H*3 H -0.15575 0.04611 0.56939
N4 N -0.34646 0.04942 0.50129
H*5 H -0.39300 0.08467 0.55930
H*6 H -0.39560 0.12655 0.44636
H*7 H -0.19514 0.27991 0.52710
C1+ C 0.05095 0.04228 0.25637
N'2+ N 0.02248 0.03417 0.34577
C3+ C 0.18725 0.04521 0.22630
C4+ C 0.43970 0.05715 0.17609
N'5+ N -0.11309 0.03439 0.34358
N'6+ N -0.17355 0.04367 0.25720
N7+ N -0.07201 0.04839 0.20063
N'8+ N 0.20126 0.01987 0.13513
N9+ N 0.32964 0.02654 0.11219
N10+ N 0.41706 0.07388 0.26716
N'11+ N 0.29169 0.07097 0.29448
O12+ O -0.09356 0.05986 0.11302
O13+ O 0.52159 0.09330 0.32569
O14+ O 0.35383 0.00226 0.02870
N15+ N 0.56920 0.07254 0.14971
H*16+ H 0.64453 0.04996 0.20189
H*17+ H 0.57903 0.01453 0.08594

#END

data_3c_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                 8.030
_cell_length_b                 13.792
_cell_length_c                 8.556
_cell_angle_alpha               90.00
_cell_angle_beta                83.99
_cell_angle_gamma                 90.00
_cell_volume                   942.367
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.41237 0.63468 0.44072
H*2 H 0.52198 0.62633 0.49164
H*3 H 0.32039 0.60013 0.51287
N4 N 0.43046 0.58491 0.29087
H*5 H 0.32051 0.59261 0.24191
H*6 H 0.52325 0.61896 0.22056
H*7 H 0.38403 0.70764 0.43742
C1+ C -0.07549 0.51572 0.32158
N'2+ N -0.21497 0.51355 0.42530
C3+ C 0.00342 0.43194 0.24518
C4+ C 0.14490 0.27516 0.11337
N'5+ N -0.24585 0.60446 0.46754
N'6+ N -0.13252 0.66514 0.39703
N7+ N -0.02344 0.61084 0.30374
N'8+ N 0.12541 0.44565 0.12559
N9+ N 0.19393 0.36527 0.06175
N10+ N 0.01667 0.26761 0.23089
N'11+ N -0.05553 0.34475 0.30067
O12+ O 0.10253 0.64577 0.22030
O13+ O -0.03152 0.18297 0.27215
O14+ O 0.30797 0.37030 -0.05211
N15+ N 0.22293 0.19448 0.05024
H*16+ H 0.15590 0.13269 0.07061
H*17+ H 0.28851 0.20583 -0.05592

#END

data_3c_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                 11.504
_cell_length_b                 13.775
_cell_length_c                 5.770
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   914.358
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.05099 0.46800 -0.49281
H*2 H -0.00123 0.51012 -0.60157
H*3 H -0.01834 0.39861 -0.50290
N4 N -0.16872 0.46682 -0.58158
H*5 H -0.21724 0.42399 -0.47415
H*6 H -0.20003 0.53614 -0.57339
H*7 H -0.04094 0.49295 -0.32520
C1+ C 0.54790 0.28437 0.44784
N'2+ N 0.48352 0.22729 0.58950
C3+ C 0.61294 0.25054 0.25022
C4+ C 0.73331 0.18329 -0.10470
N'5+ N 0.43855 0.28569 0.74745
N'6+ N 0.47137 0.37755 0.71570
N7+ N 0.54045 0.37875 0.52688
N'8+ N 0.65789 0.31685 0.10204
N9+ N 0.71790 0.28060 -0.07479
N10+ N 0.68149 0.12114 0.04806
N'11+ N 0.62176 0.15252 0.22927
O12+ O 0.58828 0.45518 0.44887
O13+ O 0.69288 0.03090 0.01075
O14+ O 0.76244 0.33663 -0.22463
N15+ N 0.79971 0.14877 -0.28162
H*16+ H 0.78527 0.07795 -0.31928
H*17+ H 0.81249 0.19731 -0.41110

#END

data_3c_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                 5.194
```

```
_cell_length_b                 7.816
_cell_length_c                23.223
_cell_angle_alpha              90.00
_cell_angle_beta               90.00
_cell_angle_gamma              90.00
_cell_volume                  942.768
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.68384 0.36355 0.08066
H*2 H 0.69389 0.39724 0.03790
H*3 H 0.74449 0.23853 0.08336
N4 N 0.41650 0.37028 0.09821
H*5 H 0.40785 0.33482 0.14051
H*6 H 0.35696 0.49444 0.09479
H*7 H 0.80960 0.43957 0.10373
C1+ C -0.36149 0.10143 0.59230
N'2+ N -0.42520 -0.03973 0.56161
C3+ C -0.15781 0.10999 0.63435
C4+ C 0.21239 0.11531 0.71222
N'5+ N -0.61981 0.00551 0.52830
N'6+ N -0.68605 0.16860 0.53626
N7+ N -0.52518 0.23238 0.57647
N'8+ N -0.08736 0.26505 0.65498
N9+ N 0.09958 0.26325 0.69407
N10+ N 0.13650 -0.03526 0.68769
N'11+ N -0.05057 -0.04254 0.64905
O12+ O -0.53677 0.38520 0.59491
O13+ O 0.25213 -0.17026 0.70347
O14+ O 0.18132 0.40198 0.71559
N15+ N 0.39502 0.11731 0.75423
H*16+ H 0.50460 0.01016 0.75564
H*17+ H 0.47686 0.23355 0.76039

#END
```

S23. Optimized crystal structure coordinates for 5 polymorphs of Guanidinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

```
data_3d_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                 13.718
```

```
_cell_length_b                 11.712
_cell_length_c                 5.005
_cell_angle_alpha               90.00
_cell_angle_beta                39.49
_cell_angle_gamma                 90.00
_cell_volume                   511.381
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.65840 0.51180 0.50501
N2 N 0.60010 0.43781 0.45199
H*3 H 0.53432 0.46447 0.43706
H*4 H 0.62012 0.35309 0.42529
N5 N 0.63002 0.62348 0.53941
H*6 H 0.67294 0.68083 0.57963
H*7 H 0.56483 0.65377 0.52620
N8 N 0.74508 0.47411 0.52363
H*9 H 0.76794 0.39010 0.49834
H*10 H 0.79025 0.52854 0.56353
C1+ C -0.28257 0.05129 0.48198
N'2+ N -0.37240 0.01817 0.46532
C3+ C -0.21028 -0.02493 0.51679
C4+ C -0.08543 -0.16905 0.59495
N'5+ N -0.41558 0.11292 0.43482
N'6+ N -0.35892 0.20562 0.43391
N7+ N -0.27403 0.16898 0.46259
N'8+ N -0.10397 0.01780 0.46166
N9+ N -0.04329 -0.05698 0.50280
N10+ N -0.18947 -0.20613 0.63052
N'11+ N -0.25552 -0.13584 0.59806
O12+ O -0.20452 0.23567 0.47489
O13+ O -0.22179 -0.31171 0.69817
O14+ O 0.05848 -0.02572 0.45270
N15+ N -0.02623 -0.24222 0.65397
H*16+ H -0.03759 -0.32569 0.62862
H*17+ H 0.07177 -0.21403 0.53303

#END

data_3d_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 13.663
_cell_length_b 11.726
_cell_length_c 12.628
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 2023.16
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.40890 -0.37984 -0.11346
N2 N 0.38977 -0.26845 -0.12284
H*3 H 0.44372 -0.21138 -0.13656
H*4 H 0.32079 -0.23808 -0.11648
N5 N 0.50090 -0.41763 -0.12223
H*6 H 0.51696 -0.50144 -0.11541
H*7 H 0.55703 -0.36349 -0.13594
N8 N 0.33604 -0.45344 -0.09530
H*9 H 0.26601 -0.42671 -0.08841
H*10 H 0.34888 -0.53795 -0.08795
C1+ C -0.03660 0.16000 0.61033
N'2+ N -0.13055 0.12665 0.59569
C3+ C 0.04541 0.08396 0.62332
C4+ C 0.19186 -0.06002 0.65019
N'5+ N -0.18246 0.22129 0.58750
N'6+ N -0.12676 0.31410 0.59686
N7+ N -0.03407 0.27769 0.61116
N'8+ N 0.13699 0.12787 0.62004
N9+ N 0.20903 0.05312 0.63375
N10+ N 0.09739 -0.09803 0.64852
N'11+ N 0.02228 -0.02790 0.63650
O12+ O 0.03814 0.34447 0.62420
O13+ O 0.08359 -0.20435 0.65938
O14+ O 0.29747 0.08550 0.63091
N15+ N 0.26709 -0.13338 0.66880
H*16+ H 0.24976 -0.21640 0.65686
H*17+ H 0.33326 -0.10324 0.64581

#END

data_3d_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                14.718
_cell_length_b                11.914
_cell_length_c                6.311
_cell_angle_alpha              90.00
_cell_angle_beta               67.85
_cell_angle_gamma                90.00
_cell_volume                  1024.97
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.41011 -0.11912 -0.14165
N2 N 0.39213 -0.22942 -0.11949
H*3 H 0.32312 -0.25928 -0.04326
H*4 H 0.44704 -0.28614 -0.17834
N5 N 0.33600 -0.04596 -0.06215
H*6 H 0.34796 0.03773 -0.07711
H*7 H 0.26589 -0.07221 0.01521
N8 N 0.50219 -0.08198 -0.24331
H*9 H 0.55925 -0.13581 -0.30458
H*10 H 0.51740 0.00100 -0.26182
C1+ C -0.03850 0.16609 0.77065
N'2+ N -0.13379 0.13457 0.84210
C3+ C 0.04385 0.09023 0.70016
C4+ C 0.19118 -0.05350 0.58061
N'5+ N -0.18554 0.22831 0.89057
N'6+ N -0.12839 0.31877 0.85544
N7+ N -0.03494 0.28173 0.77904
N'8+ N 0.13527 0.13305 0.59790
N9+ N 0.20775 0.05847 0.53973
N10+ N 0.09648 -0.09027 0.67702
N'11+ N 0.02105 -0.02030 0.74139
O12+ O 0.03880 0.34632 0.73089
O13+ O 0.08282 -0.19527 0.70415
O14+ O 0.29599 0.08995 0.44078
N15+ N 0.26728 -0.12699 0.52844
H*16+ H 0.24826 -0.20790 0.51772
H*17+ H 0.33148 -0.09655 0.41502

#END

data_3d_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                   11.891
_cell_length_b                   13.640
_cell_length_c                   6.323
_cell_angle_alpha                 90.00
_cell_angle_beta                  91.54
_cell_angle_gamma                    90.00
_cell_volume                     1025.18
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.61739 0.59045 0.76657
N2 N 0.54498 0.66413 0.79355
H*3 H 0.46120 0.65210 0.79714
H*4 H 0.57194 0.73400 0.81113
N5 N 0.57934 0.49869 0.74370
H*6 H 0.63259 0.44195 0.72314
H*7 H 0.49623 0.48342 0.74632
N8 N 0.72785 0.60852 0.76246
H*9 H 0.75838 0.67730 0.77943
H*10 H 0.78400 0.55393 0.74226
C1+ C -0.16278 0.46219 0.22306
N'2+ N -0.13131 0.36779 0.19441
C3+ C -0.08667 0.54409 0.24335
C4+ C 0.05754 0.69034 0.28652
N'5+ N -0.22529 0.31617 0.18390
N'6+ N -0.31586 0.37250 0.20583
N7+ N -0.27864 0.46531 0.23042
N'8+ N -0.12956 0.63600 0.23679
N9+ N -0.05474 0.70793 0.25883
N10+ N 0.09434 0.59552 0.28354
N'11+ N 0.02414 0.52051 0.26473
O12+ O -0.34326 0.53809 0.25804
O13+ O 0.19959 0.58128 0.30035
O14+ O -0.08627 0.79664 0.25266
N15+ N 0.13129 0.76552 0.31832
H*16+ H 0.21229 0.74764 0.29082
H*17+ H 0.10069 0.83172 0.27232

#END
```

```
data_3d_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                 17.663
_cell_length_b                 11.856
_cell_length_c                 30.743
_cell_angle_alpha               90.00
_cell_angle_beta                9.45
_cell_angle_gamma                 90.00
_cell_volume                   1057.03
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.23994 0.20605 0.46437
N2 N 0.25272 0.31675 0.44888
H*3 H 0.31604 0.34626 0.38274
H*4 H 0.19944 0.37413 0.50286
N5 N 0.31173 0.13201 0.39157
H*6 H 0.30361 0.04801 0.40170
H*7 H 0.37621 0.15790 0.32431
N8 N 0.15536 0.16939 0.55266
H*9 H 0.10017 0.22388 0.60867
H*10 H 0.14417 0.08612 0.56594
C1+ C 0.67390 0.25148 0.05877
N'2+ N 0.51213 0.22066 0.19003
C3+ C 0.77359 0.17491 -0.03290
C4+ C 0.96392 0.02970 -0.20335
N'5+ N 0.46792 0.31489 0.23764
N'6+ N 0.59621 0.40495 0.14196
N7+ N 0.72724 0.36718 0.02821
N'8+ N 0.86133 0.21805 -0.12255
N9+ N 0.95549 0.14272 -0.20667
N10+ N 0.85487 -0.00710 -0.10073
N'11+ N 0.76325 0.06352 -0.01659
O12+ O 0.87581 0.43116 -0.08602
O13+ O 0.84548 -0.11282 -0.08917
O14+ O 1.03754 0.17448 -0.29176
N15+ N 1.08235 -0.04481 -0.30222
H*16+ H 0.98224 -0.12514 -0.23938
H*17+ H 1.05748 -0.01298 -0.31862
```

#END

S24. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

```
data_3e_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                 27.604
_cell_length_b                 8.970
_cell_length_c                 4.518
_cell_angle_alpha               90.00
_cell_angle_beta                97.22
_cell_angle_gamma                 90.00
_cell_volume                   1109.82
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.09350 0.14513 -0.05474
N2 N -0.13659 0.07459 -0.09930
H*3 H -0.16473 0.10518 0.01033
H*4 H -0.14212 -0.01132 -0.24412
N5 N -0.08762 0.25915 0.14029
H*6 H -0.11575 0.29043 0.25113
N7 N -0.05649 0.10479 -0.19913
H*8 H -0.05950 0.01987 -0.34700
H*9 H -0.02467 0.16193 -0.15709
N10 N -0.04254 0.33240 0.18590
H*11 H -0.04668 0.44191 0.12863
H*12 H -0.02762 0.32268 0.40297
C1+ C 0.60502 0.19012 -0.15638
N'2+ N 0.55754 0.15465 -0.14691
C3+ C 0.64602 0.11371 0.00537
C4+ C 0.71942 -0.02793 0.31559
N'5+ N 0.53178 0.25062 -0.32423
N'6+ N 0.56027 0.34695 -0.44609
N7+ N 0.60682 0.31092 -0.34398
N'8+ N 0.69142 0.14468 -0.06110
N9+ N 0.72753 0.07143 0.09892
N10+ N 0.67235 -0.05684 0.36124
N'11+ N 0.63479 0.01353 0.21203
```

O12+ O 0.64358 0.38183 -0.41362
O13+ O 0.66563 -0.15448 0.55499
O14+ O 0.77135 0.09137 0.05161
N15+ N 0.75737 -0.09590 0.48462
H*16+ H 0.74780 -0.18911 0.58985
H*17+ H 0.78908 -0.09307 0.39346

#END

data_3e_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 7.836
_cell_length_b 26.602
_cell_length_c 5.266
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1097.71
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.42566 0.42400 0.03746
N2 N 0.35767 0.37797 0.01649
H*3 H 0.38470 0.35060 0.14327
H*4 H 0.27732 0.36937 -0.12704
N5 N 0.53223 0.43394 0.23162
H*6 H 0.55990 0.40662 0.35961
N7 N 0.39002 0.45999 -0.12949
H*8 H 0.31072 0.45397 -0.27752
H*9 H 0.44493 0.49416 -0.10477
N10 N 0.60286 0.48209 0.25252
H*11 H 0.56679 0.49832 0.41926
H*12 H 0.73248 0.48025 0.24153
C1+ C 0.00061 -0.13470 0.23864
N'2+ N -0.09296 -0.15747 0.05555
C3+ C 0.09437 -0.16046 0.43484
C4+ C 0.25856 -0.20993 0.79420
N'5+ N -0.15781 -0.12097 -0.08454
N'6+ N -0.11168 -0.07574 0.00015
N7+ N -0.01106 -0.08337 0.20431

```
N'8+ N 0.20439 -0.13375 0.57997
N9+ N 0.28504 -0.15977 0.75892
N10+ N 0.15002 -0.23446 0.63351
N'11+ N 0.06423 -0.21065 0.45345
O12+ O 0.05398 -0.04795 0.33397
O13+ O 0.13323 -0.28151 0.66319
O14+ O 0.39210 -0.13832 0.90306
N15+ N 0.33731 -0.23497 0.98665
H*16+ H 0.33967 -0.27278 0.96370
H*17+ H 0.44066 -0.21687 1.05744

#END

data_3e_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                 28.128
_cell_length_b                 4.481
_cell_length_c                 8.927
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   1125.17
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.09669 0.15734 -0.57146
N2 N -0.13930 0.18759 -0.63677
H*3 H -0.16776 0.06912 -0.60167
H*4 H -0.14414 0.33007 -0.72310
N5 N -0.09172 -0.03504 -0.45666
H*6 H -0.12017 -0.15471 -0.42087
N7 N -0.05925 0.31335 -0.61773
H*8 H -0.06158 0.45970 -0.70342
H*9 H -0.02782 0.28192 -0.56438
N10 N -0.04712 -0.06568 -0.38890
H*11 H -0.04899 -0.00762 -0.27874
H*12 H -0.03526 -0.27942 -0.39941
C1+ C 0.60812 0.04661 -0.52596
N'2+ N 0.56211 -0.00278 -0.56324
C3+ C 0.64854 -0.08210 -0.60128
```

```
C4+ C 0.72093 -0.33336 -0.74099
N'5+ N 0.53642 0.15442 -0.46774
N'6+ N 0.56357 0.30125 -0.37000
N7+ N 0.60912 0.23733 -0.40457
N'8+ N 0.69245 0.02302 -0.56861
N9+ N 0.72809 -0.10805 -0.64092
N10+ N 0.67535 -0.41889 -0.77166
N'11+ N 0.63833 -0.29993 -0.70228
O12+ O 0.64448 0.33843 -0.33206
O13+ O 0.66951 -0.61991 -0.86995
O14+ O 0.77054 -0.02358 -0.61939
N15+ N 0.75836 -0.47197 -0.80794
H*16+ H 0.74957 -0.58614 -0.90190
H*17+ H 0.78901 -0.35346 -0.80401

#END

data_3e_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                 16.447
_cell_length_b                 10.622
_cell_length_c                 6.493
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   1134.33
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.35426 0.57826 0.19245
N2 N 0.33143 0.48072 0.07507
H*3 H 0.32964 0.48744 -0.08008
H*4 H 0.31535 0.39759 0.13868
N5 N 0.37524 0.68748 0.10160
H*6 H 0.37357 0.69485 -0.05417
N7 N 0.35660 0.56931 0.39661
H*8 H 0.34132 0.48901 0.47028
H*9 H 0.37433 0.64599 0.47815
N10 N 0.39904 0.78903 0.22501
H*11 H 0.45719 0.81474 0.19127
```

H*12 H 0.36065 0.86318 0.20404
C1+ C -0.24211 0.55010 0.28818
N'2+ N -0.32338 0.52978 0.28260
C3+ C -0.18101 0.45284 0.28604
C4+ C -0.07232 0.26996 0.28871
N'5+ N -0.35770 0.64219 0.28730
N'6+ N -0.30260 0.73406 0.29709
N7+ N -0.22893 0.67833 0.29742
N'8+ N -0.10233 0.48626 0.25845
N9+ N -0.04919 0.39198 0.26045
N10+ N -0.15326 0.24377 0.30793
N'11+ N -0.20918 0.33339 0.30969
O12+ O -0.16243 0.73882 0.30807
O13+ O -0.17351 0.12903 0.32504
O14+ O 0.02588 0.41327 0.23373
N15+ N -0.01599 0.17636 0.29939
H*16+ H -0.03904 0.08915 0.27512
H*17+ H 0.03881 0.20012 0.23960

#END

data_3e_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 9.756
_cell_length_b 6.702
_cell_length_c 19.042
_cell_angle_alpha 90.00
_cell_angle_beta 83.30
_cell_angle_gamma 90.00
_cell_volume 1236.55
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.72054 -0.47574 0.52761
N2 N 0.67378 -0.58635 0.58397
H*3 H 0.67759 -0.73696 0.58238
H*4 H 0.63334 -0.52198 0.62972
N5 N 0.77369 -0.56736 0.46762
H*6 H 0.77781 -0.71859 0.46567
N7 N 0.71548 -0.27755 0.52977

H*8 H 0.67637 -0.20352 0.57378
H*9 H 0.75227 -0.20100 0.48561
N10 N 0.82237 -0.45103 0.40892
H*11 H 0.92489 -0.47639 0.39502
H*12 H 0.76835 -0.48196 0.36757
C1+ C 0.51606 -0.01543 0.26354
N'2+ N 0.48822 -0.01215 0.19551
C3+ C 0.65246 -0.01850 0.28557
C4+ C 0.90506 -0.03083 0.32225
N'5+ N 0.35231 -0.01035 0.19809
N'6+ N 0.29103 -0.01372 0.26443
N7+ N 0.39238 -0.01656 0.30691
N'8+ N 0.66608 0.01108 0.35474
N9+ N 0.79455 0.00409 0.37142
N10+ N 0.88286 -0.05190 0.25315
N'11+ N 0.75741 -0.04886 0.23314
O12+ O 0.37007 -0.02251 0.37395
O13+ O 0.98788 -0.07555 0.20800
O14+ O 0.81841 0.03207 0.43468
N15+ N 1.03455 -0.04614 0.34164
H*16+ H 1.11061 -0.02812 0.30114
H*17+ H 1.04445 0.01378 0.38964

#END

S25. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

data_3f_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 27.390
_cell_length_b 11.978
_cell_length_c 7.137
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 2341.49
loop_
_atom_site_label

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.07443 0.23836 -0.03338
N2 N -0.12314 0.23309 -0.02058
H*3 H -0.13896 0.15644 -0.02784
N4 N -0.04878 0.14320 -0.05506
H*5 H -0.01187 0.14635 -0.06489
N6 N -0.05169 0.33657 -0.02476
H*7 H -0.07245 0.40597 -0.00838
H*8 H -0.01503 0.34293 -0.03403
N9 N -0.07387 0.04146 -0.06356
N10 N -0.14961 0.33231 0.00195
H*11 H -0.16867 0.32991 0.12441
H*12 H -0.06771 0.00336 -0.18887
H*13 H -0.06330 -0.00922 0.04353
H*14 H -0.17306 0.34246 -0.10745
C1+ C 0.62158 0.21869 0.11970
N'2+ N 0.62803 0.10680 0.10805
C3+ C 0.65972 0.29853 0.15715
C4+ C 0.73099 0.43995 0.23255
N'5+ N 0.58452 0.06415 0.07249
N'6+ N 0.55025 0.14293 0.06191
N7+ N 0.57276 0.24156 0.09089
N'8+ N 0.64989 0.40849 0.13494
N9+ N 0.68655 0.47742 0.17390
N10+ N 0.73844 0.32745 0.24477
N'11+ N 0.70332 0.25441 0.21012
O12+ O 0.55056 0.33466 0.09246
O13+ O 0.78072 0.29458 0.29174
O14+ O 0.68121 0.58193 0.15559
N15+ N 0.76702 0.51298 0.27952
H*16+ H 0.80084 0.47874 0.28090
H*17+ H 0.76198 0.59093 0.22785

#END

data_3f_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                  27.593
_cell_length_b                  4.333
_cell_length_c                  9.788
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
_cell_volume                   1170.26
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.08935 0.53256 -0.21887
N2 N -0.08582 0.71142 -0.10779
H*3 H -0.11438 0.85054 -0.08513
N4 N -0.13003 0.54427 -0.29492
H*5 H -0.13304 0.40963 -0.37926
N6 N -0.05304 0.34555 -0.25355
H*7 H -0.02314 0.34432 -0.19336
H*8 H -0.05476 0.20834 -0.33674
N9 N -0.16747 0.74344 -0.25547
N10 N -0.04343 0.69824 -0.02912
H*11 H -0.05155 0.62959 0.06772
H*12 H -0.17389 0.90206 -0.33004
H*13 H -0.19817 0.62133 -0.23530
H*14 H -0.02733 0.90966 -0.02679
C1+ C 0.60214 0.28564 -0.16381
N'2+ N 0.55452 0.22206 -0.18214
C3+ C 0.64077 0.17863 -0.25088
C4+ C 0.70992 -0.03372 -0.41184
N'5+ N 0.53138 0.36137 -0.08135
N'6+ N 0.56175 0.50999 0.00169
N7+ N 0.60677 0.46627 -0.04837
N'8+ N 0.68562 0.29943 -0.23409
N9+ N 0.71958 0.18776 -0.31676
N10+ N 0.66331 -0.13524 -0.42556
N'11+ N 0.62794 -0.03618 -0.34542
O12+ O 0.64472 0.57431 0.00737
O13+ O 0.65486 -0.33143 -0.51872
O14+ O 0.76264 0.28821 -0.31017
N15+ N 0.74597 -0.15318 -0.49058
H*16+ H 0.73403 -0.26162 -0.57588
H*17+ H 0.77611 -0.01985 -0.49441

#END

data_3f_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 10.735
_cell_length_b 27.516
_cell_length_c 4.329
_cell_angle_alpha 90.00
_cell_angle_beta 68.80
_cell_angle_gamma 90.00
_cell_volume 1192.18
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.86856 0.40984 -0.42425
N2 N 0.75818 0.41341 -0.49846
H*3 H 0.73683 0.38542 -0.62443
N4 N 0.94563 0.36987 -0.51828
H*5 H 1.02944 0.36684 -0.46317
N6 N 0.90154 0.44542 -0.25946
H*7 H 0.84062 0.47481 -0.19372
H*8 H 0.98416 0.44367 -0.20034
N9 N 0.90796 0.33319 -0.69109
N10 N 0.67843 0.45506 -0.40004
H*11 H 0.58494 0.44562 -0.24536
H*12 H 0.97991 0.32839 -0.91901
H*13 H 0.89147 0.30152 -0.56081
H*14 H 0.67319 0.47243 -0.60272
C1+ C 0.81180 0.10217 -0.10976
N'2+ N 0.82979 0.05474 -0.05329
C3+ C 0.90003 0.14114 -0.10020
C4+ C 1.06340 0.21100 -0.06770
N'5+ N 0.72789 0.03116 -0.08499
N'6+ N 0.64449 0.06107 -0.15688
N7+ N 0.69544 0.10623 -0.17465
N'8+ N 0.88229 0.18547 -0.21358
N9+ N 0.96622 0.21980 -0.19395
N10+ N 1.07769 0.16482 0.03024
N'11+ N 0.99647 0.12913 0.02085
O12+ O 0.63975 0.14388 -0.23551
O13+ O 1.17250 0.15710 0.13328
O14+ O 0.95881 0.26242 -0.29694
N15+ N 1.14368 0.24750 -0.03709
H*16+ H 1.22893 0.23581 -0.01151
H*17+ H 1.14545 0.27693 -0.17928

#END

data_3f_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                   13.239
_cell_length_b                   11.963
_cell_length_c                   7.572
_cell_angle_alpha                 90.00
_cell_angle_beta                  78.66
_cell_angle_gamma                   90.00
_cell_volume                     1175.83
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.34201 0.23805 0.53543
N2 N 0.24150 0.23330 0.53105
H*3 H 0.20695 0.15705 0.54542
N4 N 0.39245 0.14293 0.55837
H*5 H 0.46860 0.14570 0.56186
N6 N 0.39135 0.33572 0.51731
H*7 H 0.35033 0.40511 0.50035
H*8 H 0.46707 0.34168 0.52010
N9 N 0.33818 0.04177 0.57697
N10 N 0.18947 0.33248 0.50717
H*11 H 0.13139 0.34561 0.61515
H*12 H 0.36870 -0.01164 0.47582
H*13 H 0.33989 0.00650 0.69871
H*14 H 0.16013 0.32751 0.39278
C1+ C -0.26134 0.21783 0.11038
N'2+ N -0.24915 0.10539 0.10535
C3+ C -0.18584 0.29687 0.14675
C4+ C -0.04560 0.43688 0.22029
N'5+ N -0.33508 0.06381 0.06839
N'6+ N -0.40245 0.14384 0.05055
N7+ N -0.35759 0.24216 0.07612
N'8+ N -0.20083 0.40689 0.11898
N9+ N -0.12881 0.47509 0.15716
N10+ N -0.03431 0.32423 0.23833
N'11+ N -0.10381 0.25192 0.20466
O12+ O -0.40134 0.33624 0.07061
O13+ O 0.04602 0.29049 0.28978
O14+ O -0.13518 0.57955 0.13389
N15+ N 0.02423 0.50936 0.26590
H*16+ H 0.09280 0.47375 0.27268
```

```
H*17+ H 0.02204 0.58661 0.21192

#END

data_3f_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                 15.863
_cell_length_b                 11.955
_cell_length_c                 7.603
_cell_angle_alpha               90.00
_cell_angle_beta               121.96
_cell_angle_gamma                90.00
_cell_volume                   1223.29
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.35206 0.24062 0.83625
N2 N 0.25423 0.23770 0.75969
H*3 H 0.21955 0.16232 0.71338
N4 N 0.39979 0.14489 0.84854
H*5 H 0.47391 0.14628 0.90633
N6 N 0.40143 0.33708 0.89937
H*7 H 0.36250 0.40698 0.88723
H*8 H 0.47517 0.34165 0.95768
N9 N 0.34558 0.04504 0.78079
N10 N 0.20501 0.33749 0.74728
H*11 H 0.17373 0.33126 0.83431
H*12 H 0.34943 0.01167 0.66203
H*13 H 0.37184 -0.01056 0.89994
H*14 H 0.15136 0.35344 0.59696
C1+ C -0.25553 0.22283 0.62425
N'2+ N -0.24235 0.11062 0.63091
C3+ C -0.17971 0.30495 0.67264
C4+ C -0.03654 0.45088 0.77011
N'5+ N -0.32893 0.06566 0.57654
N'6+ N -0.39718 0.14330 0.53651
N7+ N -0.35270 0.24354 0.56514
N'8+ N -0.20668 0.41359 0.62749
N9+ N -0.13286 0.48485 0.67837
N10+ N -0.01610 0.33919 0.80350
```

N'11+ N -0.08598 0.26404 0.75870
O12+ O -0.39650 0.33624 0.54234
O13+ O 0.07347 0.30923 0.88071
O14+ O -0.15050 0.58831 0.64051
N15+ N 0.03779 0.52660 0.82886
H*16+ H 0.10156 0.49301 0.85213
H*17+ H 0.01414 0.60197 0.75846

#END

S26. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidinium 6-amino-3-(1-hydroxy-1*H*-tetrazolate-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (ionic form).

data_3g_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 14.108
_cell_length_b 12.007
_cell_length_c 7.410
_cell_angle_alpha 90.00
_cell_angle_beta 95.62
_cell_angle_gamma 90.00
_cell_volume 1249.18
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.35662 0.22537 0.04798
N2 N 0.29774 0.31199 0.06124
H*3 H 0.32754 0.38745 0.09291
N4 N 0.32101 0.12402 0.00654
H*5 H 0.24901 0.11632 -0.01380
N6 N 0.45110 0.24010 0.07616
H*7 H 0.49331 0.17234 0.06483
N8 N 0.38406 0.03485 -0.00651
N9 N 0.19927 0.29441 0.03116
H*10 H 0.17138 0.34173 -0.07511
H*11 H 0.37169 -0.02497 0.08575
H*12 H 0.37547 0.00202 -0.13378
H*13 H 0.16760 0.31474 0.14442
N14 N 0.48653 0.34686 0.11929
H*15 H 0.52489 0.34586 0.24307

H*16 H 0.52867 0.37285 0.02353
C1+ C -0.23393 0.21049 0.34695
N'2+ N -0.21375 0.10093 0.32980
C3+ C -0.16802 0.30033 0.32698
C4+ C -0.04279 0.46070 0.29467
N'5+ N -0.29238 0.04662 0.35811
N'6+ N -0.36213 0.11568 0.39394
N7+ N -0.32705 0.21994 0.38735
N'8+ N -0.20162 0.40599 0.31832
N9+ N -0.13677 0.48471 0.30195
N10+ N -0.01531 0.35160 0.29763
N'11+ N -0.07610 0.26933 0.31588
O12+ O -0.37472 0.30660 0.41733
O13+ O 0.07178 0.33121 0.28271
O14+ O -0.16117 0.58623 0.29076
N15+ N 0.02240 0.54359 0.28627
H*16+ H 0.08456 0.51821 0.24193
H*17+ H -0.00637 0.61777 0.24517

#END

data_3g_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 13.907
_cell_length_b 11.983
_cell_length_c 7.420
_cell_angle_alpha 90.00
_cell_angle_beta 80.06
_cell_angle_gamma 90.00
_cell_volume 1217.96
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.15227 0.22208 0.48222
N2 N -0.21394 0.30858 0.48928
H*3 H -0.18497 0.38481 0.45249
N4 N -0.18668 0.11974 0.52929
H*5 H -0.25996 0.11121 0.56955
N6 N -0.05619 0.23792 0.42810
H*7 H -0.01188 0.17021 0.42462

N8 N -0.12071 0.03071 0.52074
N9 N -0.31403 0.28983 0.54630
H*10 H -0.35124 0.31147 0.44478
H*11 H -0.12431 -0.00394 0.64705
H*12 H -0.13672 -0.02807 0.43131
H*13 H -0.33883 0.33560 0.66052
N14 N -0.02207 0.34570 0.37962
H*15 H 0.02495 0.37077 0.46270
H*16 H 0.01253 0.34665 0.24696
C1+ C 0.26310 0.20383 0.13391
N'2+ N 0.28210 0.09321 0.14108
C3+ C 0.32864 0.29157 0.16756
C4+ C 0.45080 0.44808 0.23685
N'5+ N 0.20424 0.04158 0.10234
N'6+ N 0.13563 0.11341 0.07177
N7+ N 0.17112 0.21670 0.09053
N'8+ N 0.30745 0.39792 0.12700
N9+ N 0.37043 0.47465 0.16339
N10+ N 0.46877 0.33828 0.26752
N'11+ N 0.40840 0.25795 0.23631
O12+ O 0.12371 0.30544 0.07254
O13+ O 0.54623 0.31530 0.32844
O14+ O 0.35769 0.57657 0.12853
N15+ N 0.51137 0.52919 0.28025
H*16+ H 0.57826 0.50104 0.29505
H*17+ H 0.50462 0.60304 0.21711

#END

data_3g_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 12.027
_cell_length_b 6.879
_cell_length_c 29.103
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 2407.8
loop_

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.27146 -0.04218 -0.42625
N2 N 0.25490 -0.06318 -0.47153
H*3 H 0.32280 -0.05973 -0.49232
N4 N 0.18475 -0.04563 -0.39732
H*5 H 0.10781 -0.06449 -0.41107
N6 N 0.37473 -0.01772 -0.40990
H*7 H 0.38377 -0.00233 -0.37536
N8 N 0.20426 -0.02336 -0.35014
N9 N 0.14617 -0.08854 -0.48775
H*10 H 0.13961 -0.21845 -0.50432
H*11 H 0.16372 0.09650 -0.33826
H*12 H 0.17732 -0.14327 -0.33289
H*13 H 0.12601 0.02132 -0.50968
N14 N 0.46395 -0.01464 -0.44086
H*15 H 0.50425 0.11529 -0.43886
H*16 H 0.51785 -0.12448 -0.43349
C1+ C -0.29074 0.17482 0.13228
N'2+ N -0.40047 0.16394 0.14244
C3+ C -0.20295 0.19850 0.16552
C4+ C -0.04651 0.24858 0.22804
N'5+ N -0.45251 0.14291 0.10277
N'6+ N -0.38185 0.14102 0.06748
N7+ N -0.27887 0.16059 0.08522
N'8+ N -0.09636 0.17556 0.15160
N9+ N -0.01967 0.20162 0.18391
N10+ N -0.15627 0.26206 0.23964
N'11+ N -0.23665 0.24008 0.20901
O12+ O -0.19127 0.16683 0.06088
O13+ O -0.17919 0.29755 0.28134
O14+ O 0.08252 0.18136 0.17447
N15+ N 0.03422 0.28301 0.25976
H*16+ H 0.00748 0.27421 0.29271
H*17+ H 0.10966 0.22896 0.25098

#END

data_3g_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                 11.507
_cell_length_b                 14.293
_cell_length_c                 8.584
_cell_angle_alpha               90.00
_cell_angle_beta                117.52
_cell_angle_gamma                90.00
_cell_volume                   1252.06
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.47720 0.40229 0.59023
N2 N 0.48940 0.34350 0.47697
H*3 H 0.40977 0.33391 0.35833
N4 N 0.57924 0.41744 0.74850
H*5 H 0.66413 0.38301 0.77759
N6 N 0.36296 0.44593 0.54522
H*7 H 0.35769 0.48994 0.63477
N8 N 0.56397 0.47921 0.86450
N9 N 0.60984 0.29875 0.52716
H*10 H 0.64633 0.31652 0.44338
H*11 H 0.57999 0.44490 0.97663
H*12 H 0.62832 0.53332 0.89419
H*13 H 0.59800 0.22810 0.52583
N14 N 0.25779 0.42891 0.37903
H*15 H 0.18112 0.40123 0.39189
H*16 H 0.22945 0.48966 0.30945
C1+ C 0.34545 0.03666 0.25819
N'2+ N 0.22101 0.05437 0.22738
C3+ C 0.38361 -0.03713 0.17677
C4+ C 0.44732 -0.17561 0.02735
N'5+ N 0.22804 0.12680 0.32698
N'6+ N 0.35100 0.15631 0.42149
N7+ N 0.42726 0.10056 0.38014
N'8+ N 0.50753 -0.03768 0.19729
N9+ N 0.53638 -0.10826 0.12035
N10+ N 0.32292 -0.16802 0.00756
N'11+ N 0.28826 -0.10010 0.08249
O12+ O 0.55102 0.10865 0.44849
O13+ O 0.24035 -0.22927 -0.08591
O14+ O 0.64942 -0.11454 0.13020
N15+ N 0.48182 -0.24927 -0.04295
H*16+ H 0.40467 -0.28306 -0.13922
H*17+ H 0.56439 -0.23830 -0.05476

#END

data_3g_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                   12.119
_cell_length_b                   28.013
_cell_length_c                   3.924
_cell_angle_alpha                 90.00
_cell_angle_beta                 114.24
_cell_angle_gamma                   90.00
_cell_volume                     1214.71
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.23293 0.07539 -0.66100
N2 N -0.24824 0.02816 -0.64616
H*3 H -0.17547 0.00683 -0.59783
N4 N -0.32598 0.10511 -0.72399
H*5 H -0.40665 0.09043 -0.75903
N6 N -0.12457 0.09290 -0.61285
H*7 H -0.11668 0.12891 -0.62614
N8 N -0.30764 0.15433 -0.73820
N9 N -0.36239 0.01076 -0.69739
H*10 H -0.35635 -0.00741 -0.46557
H*11 H -0.36325 0.16739 -0.99345
H*12 H -0.32478 0.17128 -0.53546
H*13 H -0.39482 -0.01129 -0.92355
N14 N -0.02876 0.06108 -0.54741
H*15 H 0.00157 0.06424 -0.75298
H*16 H 0.04004 0.06812 -0.29499
C1+ C -0.25772 -0.13285 0.92862
N'2+ N -0.36695 -0.14165 0.93352
C3+ C -0.16286 -0.16764 1.00598
C4+ C 0.00861 -0.23271 1.16299
N'5+ N -0.42672 -0.10083 0.84888
N'6+ N -0.36115 -0.06602 0.79211
N7+ N -0.25385 -0.08536 0.84012
N'8+ N -0.06630 -0.15621 0.93246
N9+ N 0.01831 -0.18975 1.01441
N10+ N -0.09384 -0.24207 1.21596
N'11+ N -0.18079 -0.21002 1.14431
O12+ O -0.16863 -0.06178 0.81084
O13+ O -0.10306 -0.28305 1.33919
O14+ O 0.11169 -0.18274 0.95223
N15+ N 0.09942 -0.26541 1.25961
```

H*16+ H 0.07357 -0.29904 1.28808
H*17+ H 0.15744 -0.25987 1.13721

#END

S27. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

data_1a_q_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 13.018
_cell_length_b 8.384
_cell_length_c 5.859
_cell_angle_alpha 90.00
_cell_angle_beta 59.20
_cell_angle_gamma 90.00
_cell_volume 549.278
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.42946 0.18951 -0.26730
H*2 H 0.39130 0.29970 -0.21466
H*3 H 0.45368 0.15886 -0.13302
H*4 H 0.36392 0.11217 -0.24133
C1+ C -0.15449 -0.27122 0.78229
N2+ N -0.17100 -0.15330 0.64747
N'3+ N -0.24011 -0.20668 0.55854
N'4+ N -0.26522 -0.35572 0.63889
N'5+ N -0.21353 -0.39845 0.77723
O6+ O -0.12786 -0.00167 0.60018
N7+ N -0.08407 -0.25969 0.91016
O8+ O -0.07921 -0.37890 1.02327
O9+ O -0.03605 -0.13052 0.89195
H*10+ H -0.15996 0.04484 0.49691

#END

data_1a_q_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                   7.730
_cell_length_b                   6.642
_cell_length_c                   10.956
_cell_angle_alpha                 90.00
_cell_angle_beta                 99.39
_cell_angle_gamma                   90.00
_cell_volume                     554.973
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.70053 0.80451 0.60261
H*2 H 0.81142 0.72037 0.62487
H*3 H 0.64370 0.76243 0.51585
H*4 H 0.61731 0.76208 0.66111
C1+ C -0.20420 0.22934 0.64855
N2+ N -0.27450 0.19050 0.75103
N'3+ N -0.43662 0.26285 0.73573
N'4+ N -0.46422 0.34482 0.62488
N'5+ N -0.32301 0.32621 0.56920
O6+ O -0.20186 0.09452 0.85665
N7+ N -0.02864 0.17402 0.62933
O8+ O 0.01245 0.22175 0.53054
O9+ O 0.06179 0.08420 0.71473
H*10+ H -0.29438 0.09750 0.90746

#END

data_1a_q_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                   8.941
_cell_length_b                   14.808
_cell_length_c                   5.814
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 133.02
_cell_angle_gamma                90.00
_cell_volume                     562.786
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.22973 0.39546 0.56300
H*2 H -0.18116 0.42381 0.76404
H*3 H -0.18804 0.43827 0.47775
H*4 H -0.14783 0.33755 0.62692
C1+ C -0.16197 0.15024 0.10719
N2+ N -0.19352 0.11495 -0.13697
N'3+ N -0.26722 0.03191 -0.19211
N'4+ N -0.28018 0.01705 0.01701
N'5+ N -0.21624 0.08893 0.20434
O6+ O -0.16012 0.15281 -0.31166
N7+ N -0.08229 0.23993 0.23914
O8+ O -0.06400 0.26030 0.46035
O9+ O -0.04089 0.28676 0.11471
H*10+ H -0.20196 0.10581 -0.46330

#END

data_1a_q_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                   8.772
_cell_length_b                   10.621
_cell_length_c                   10.814
_cell_angle_alpha                90.00
_cell_angle_beta                 34.56
_cell_angle_gamma                90.00
_cell_volume                     571.53
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.43014 0.55348 0.80380
```

H*2 H 0.40495 0.49562 0.74635
H*3 H 0.60761 0.52899 0.72564
H*4 H 0.45366 0.64238 0.75433
C1+ C -0.09019 0.51551 0.27296
N2+ N 0.01970 0.59645 0.28139
N'3+ N -0.04033 0.71333 0.28804
N'4+ N -0.18540 0.70320 0.28367
N'5+ N -0.21907 0.58225 0.27437
O6+ O 0.16965 0.57149 0.28343
N7+ N -0.06976 0.37902 0.26393
O8+ O -0.18244 0.32092 0.25703
O9+ O 0.05949 0.33515 0.26413
H*10+ H 0.20955 0.65470 0.29026

#END

data_1a_q_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 10.629
_cell_length_b 8.744
_cell_length_c 12.270
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1140.37
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.44774 0.74873 -0.15520
H*2 H 0.50480 0.66221 -0.12964
H*3 H 0.35829 0.71975 -0.13360
H*4 H 0.47121 0.84302 -0.11081
C1+ C -0.01560 -0.32695 0.38610
N2+ N -0.09653 -0.20881 0.39582
N'3+ N -0.21285 -0.26308 0.40284
N'4+ N -0.20239 -0.41286 0.39741

N'5+ N -0.08179 -0.45520 0.38708
O6+ O -0.07203 -0.05624 0.39871
N7+ N 0.12036 -0.31466 0.37632
O8+ O 0.17854 -0.43421 0.36826
O9+ O 0.16375 -0.18457 0.37710
H*10+ H -0.15505 -0.00991 0.40636

#END

S28. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

data_1b_q_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 8.753
_cell_length_b 5.408
_cell_length_c 12.262
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 580.437
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.62506 0.32067 -0.09121
H*2 H 0.67631 0.15385 -0.10522
H*3 H 0.54327 0.28777 -0.03351
O4 O 0.53853 0.36630 -0.18959
H*5 H 0.57572 0.52607 -0.21247
C1+ C -0.14825 0.55147 0.06988
N2+ N -0.23991 0.59704 0.15607
N'3+ N -0.22327 0.41699 0.22864
N'4+ N -0.12235 0.26370 0.18670
N'5+ N -0.07431 0.34232 0.08888
O6+ O -0.33687 0.78963 0.17311
N7+ N -0.13383 0.70589 -0.02665
O8+ O -0.04502 0.63520 -0.09654
O9+ O -0.21277 0.89342 -0.02856
H*10+ H -0.38132 0.75434 0.24438

```
#END

data_1b_q_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                  9.753
_cell_length_b                  14.812
_cell_length_c                  8.304
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                   90.00
_cell_volume                    1199.61
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.56359 0.49864 0.32208
H*2 H 0.60001 0.44555 0.25609
H*3 H 0.61212 0.49476 0.43096
O4 O 0.42367 0.47349 0.35796
H*5 H 0.37216 0.52426 0.31742
C1+ C 0.79646 0.16130 0.09292
N2+ N 0.81579 0.25095 0.11103
N'3+ N 0.72499 0.28245 0.21596
N'4+ N 0.65130 0.21242 0.26099
N'5+ N 0.69326 0.13692 0.18693
O6+ O 0.90961 0.30563 0.03922
N7+ N 0.87553 0.10226 -0.01172
O8+ O 0.84332 0.02277 -0.01254
O9+ O 0.96753 0.13823 -0.08954
H*10+ H 0.88982 0.36507 0.08415

#END

data_1b_q_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                 4.508
_cell_length_b                 13.218
_cell_length_c                 10.779
_cell_angle_alpha               90.00
_cell_angle_beta                70.33
_cell_angle_gamma                 90.00
_cell_volume                   604.806
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.26054 -0.29944 0.23386
H*2 H -0.15133 -0.25068 0.27821
H*3 H -0.42562 -0.33663 0.30893
O4 O -0.02442 -0.37566 0.17606
H*5 H -0.01020 -0.37489 0.08470
C1+ C 0.36532 -0.11266 0.19807
N2+ N 0.51843 -0.04516 0.24856
N'3+ N 0.38574 -0.04373 0.37870
N'4+ N 0.15419 -0.10984 0.40676
N'5+ N 0.13653 -0.15339 0.29716
O6+ O 0.76857 0.01475 0.18486
N7+ N 0.43992 -0.13615 0.05909
O8+ O 0.27536 -0.19944 0.03170
O9+ O 0.66234 -0.08982 -0.01769
H*10+ H 0.80778 0.05205 0.25589

#END

data_1b_q_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                 12.017
_cell_length_b                 8.743
_cell_length_c                 5.619
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 92.33
_cell_angle_gamma                90.00
_cell_volume                     589.87
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.32497 0.46679 -0.23877
H*2 H 0.32946 0.37322 -0.34699
H*3 H 0.38199 0.44815 -0.10191
O4 O 0.21882 0.45000 -0.12947
H*5 H 0.18217 0.54554 -0.16817
C1+ C 0.06501 0.23638 0.51024
N2+ N 0.11249 0.32792 0.34975
N'3+ N 0.03302 0.39473 0.21583
N'4+ N -0.06180 0.34401 0.29464
N'5+ N -0.04441 0.24624 0.47606
O6+ O 0.22228 0.35465 0.31703
N7+ N 0.12419 0.14351 0.68886
O8+ O 0.06723 0.06769 0.81917
O9+ O 0.22625 0.15035 0.69139
H*10+ H 0.22164 0.42692 0.18473

#END

data_1b_q_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                   10.081
_cell_length_b                   5.079
_cell_length_c                   14.743
_cell_angle_alpha                90.00
_cell_angle_beta                 50.76
_cell_angle_gamma                90.00
_cell_volume                     584.643
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

N1 N -0.42836 -0.02601 0.66320
H*2 H -0.49685 0.13355 0.67114
H*3 H -0.49556 -0.18721 0.67090
O4 O -0.45250 -0.02543 0.77086
H*5 H -0.33644 -0.02414 0.74319
C1+ C 0.13775 0.62685 0.11147
N2+ N 0.11191 0.80675 0.05667
N'3+ N -0.03818 0.76060 0.08244
N'4+ N -0.10265 0.55442 0.15227
N'5+ N 0.00326 0.46818 0.17155
O6+ O 0.21467 1.00841 -0.01460
N7+ N 0.28741 0.61125 0.10520
O8+ O 0.28853 0.43485 0.16074
O9+ O 0.39877 0.77785 0.04435
H*10+ H 0.15043 1.09114 -0.03589

#END

S29. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

data_1c_q_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 11.092
_cell_length_b 11.866
_cell_length_c 5.650
_cell_angle_alpha 90.00
_cell_angle_beta 120.34
_cell_angle_gamma 90.00
_cell_volume 641.793
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.63548 -0.08371 0.49591
H*2 H 0.58628 -0.01211 0.39206
H*3 H 0.59343 -0.10632 0.61249
N4 N 0.78249 -0.06627 0.67743
H*5 H 0.83140 -0.08231 0.56980
H*6 H 0.80457 0.01485 0.74593
C1+ C 0.53761 0.26718 -0.08302

```
N2+ N 0.43979 0.26815 -0.00801
N'3+ N 0.46650 0.18564 0.17042
N'4+ N 0.57958 0.13513 0.20313
N'5+ N 0.62551 0.18376 0.04921
O6+ O 0.32879 0.33839 -0.09008
N7+ N 0.54457 0.34448 -0.27547
O8+ O 0.64073 0.33081 -0.31848
O9+ O 0.45259 0.41639 -0.37665
H*10+ H 0.28434 0.31136 0.01046

#END

data_1c_q_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                 8.880
_cell_length_b                 20.242
_cell_length_c                 6.300
_cell_angle_alpha               90.00
_cell_angle_beta                32.80
_cell_angle_gamma                90.00
_cell_volume                   613.44
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.21032 -0.39291 -0.53410
H*2 H 0.34901 -0.43057 -0.71763
H*3 H 0.26331 -0.36800 -0.46270
N4 N -0.06886 -0.41668 -0.17632
H*5 H -0.15569 -0.42051 -0.22007
H*6 H -0.07380 -0.46234 -0.10205
C1+ C 0.50823 0.63649 -0.35639
N2+ N 0.68620 0.67127 -0.44500
N'3+ N 0.69492 0.73318 -0.52427
N'4+ N 0.52361 0.73586 -0.48396
N'5+ N 0.40584 0.67692 -0.38061
O6+ O 0.83997 0.65070 -0.45859
N7+ N 0.44166 0.56684 -0.25276
O8+ O 0.27556 0.54369 -0.18164
O9+ O 0.55951 0.53789 -0.24676
H*10+ H 0.93999 0.69036 -0.53342
```

```
#END

data_1c_q_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                 12.124
_cell_length_b                 11.060
_cell_length_c                 9.516
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1276.01
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.07462 -0.05466 0.34342
H*2 H -0.00274 -0.08943 0.38177
H*3 H -0.10060 -0.10942 0.26424
N4 N -0.05985 0.06435 0.28592
H*5 H -0.07175 0.12474 0.36504
H*6 H 0.01796 0.07689 0.24781
C1+ C 0.79366 0.14587 0.05246
N2+ N 0.78132 0.26391 0.08482
N'3+ N 0.69735 0.27585 0.17318
N'4+ N 0.65917 0.16592 0.19413
N'5+ N 0.71708 0.08413 0.12094
O6+ O 0.84074 0.36072 0.03984
N7+ N 0.87670 0.09592 -0.04127
O8+ O 0.87533 -0.01330 -0.05806
O9+ O 0.94050 0.16877 -0.09475
H*10+ H 0.80596 0.42912 0.08702

#END

data_1c_q_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                   10.477
_cell_length_b                   9.284
_cell_length_c                   6.515
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
_cell_angle_gamma                    90.00
_cell_volume                     633.704
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.71910 0.05985 0.58765
H*2 H 0.76706 0.07247 0.45257
H*3 H 0.69013 -0.04449 0.59647
N4 N 0.60715 0.14892 0.59765
H*5 H 0.63348 0.24517 0.65890
H*6 H 0.56960 0.16829 0.45585
C1+ C 0.11117 -0.12527 0.38979
N2+ N 0.04390 -0.05647 0.53675
N'3+ N 0.01405 -0.14965 0.68357
N'4+ N 0.06287 -0.27386 0.62591
N'5+ N 0.12323 -0.26177 0.44535
O6+ O 0.00809 0.08414 0.54638
N7+ N 0.16131 -0.06019 0.20348
O8+ O 0.22000 -0.13932 0.08788
O9+ O 0.13968 0.06873 0.18028
H*10+ H -0.03859 0.09055 0.67562

#END

data_1c_q_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                 5.978
_cell_length_b                 10.202
_cell_length_c                 11.454
_cell_angle_alpha               90.00
_cell_angle_beta                115.45
_cell_angle_gamma                 90.00
_cell_volume                   630.764
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.24447 0.92879 0.20673
H*2 H 0.38177 0.90234 0.18104
H*3 H 0.16867 1.01370 0.15998
N4 N 0.33767 0.95314 0.34310
H*5 H 0.33342 0.86682 0.38648
H*6 H 0.51668 0.98517 0.38210
C1+ C -0.08908 0.70143 0.11678
N2+ N -0.16707 0.73496 0.20719
N'3+ N -0.37541 0.80328 0.15141
N'4+ N -0.42312 0.81104 0.02823
N'5+ N -0.24947 0.74906 0.00433
O6+ O -0.06255 0.70788 0.33592
N7+ N 0.13248 0.62617 0.13959
O8+ O 0.17367 0.60518 0.04590
O9+ O 0.25738 0.59081 0.25144
H*10+ H -0.17471 0.74899 0.36661

#END
```

S30. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

```
data_1d_q_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                 7.403
_cell_length_b                 14.650
_cell_length_c                 7.567
_cell_angle_alpha               90.00
_cell_angle_beta                69.18
_cell_angle_gamma                 90.00
```

```
_cell_volume                    767.083
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.31524 0.44984 0.36568
N'2 N 0.26337 0.52427 0.45991
H*3 H 0.28751 0.52159 0.58445
N4 N 0.27462 0.43563 0.20145
H*5 H 0.38161 0.40500 0.09455
H*6 H 0.22313 0.49269 0.16014
N7 N 0.41479 0.37650 0.40677
H*8 H 0.42407 0.37890 0.53688
H*9 H 0.37657 0.31402 0.37429
C1+ C -0.06660 0.16585 0.43112
N2+ N -0.14072 0.24949 0.48838
N'3+ N -0.32917 0.24800 0.52149
N'4+ N -0.36877 0.16413 0.48455
N'5+ N -0.20943 0.11211 0.42857
O6+ O -0.04943 0.32647 0.51240
N7+ N 0.13499 0.13982 0.38119
O8+ O 0.17562 0.06088 0.33242
O9+ O 0.24544 0.20004 0.39297
H*10+ H -0.15283 0.37161 0.55471

#END

data_1d_q_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                  13.200
_cell_length_b                  8.917
_cell_length_c                  7.241
_cell_angle_alpha                 90.00
_cell_angle_beta                 121.69
_cell_angle_gamma                   90.00
_cell_volume                    725.222
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

```
_atom_site_fract_z
C1 C 0.69340 -0.38349 0.78073
N'2 N 0.58987 -0.32303 0.69367
H*3 H 0.58908 -0.21840 0.63585
N4 N 0.71683 -0.51948 0.89093
H*5 H 0.76765 -0.59205 0.86613
H*6 H 0.64195 -0.56717 0.87059
N7 N 0.79217 -0.32887 0.77872
H*8 H 0.78368 -0.22188 0.72605
H*9 H 0.87207 -0.34915 0.91539
C1+ C 0.19667 0.87049 0.27458
N2+ N 0.11208 0.95185 0.28013
N'3+ N 0.01159 0.87363 0.18771
N'4+ N 0.03517 0.74597 0.12673
N'5+ N 0.14864 0.74119 0.17837
O6+ O 0.11998 1.09123 0.36282
N7+ N 0.31894 0.91738 0.35970
O8+ O 0.38300 0.82875 0.34021
O9+ O 0.34610 1.04222 0.44339
H*10+ H 0.04025 1.10949 0.33497

#END

data_1d_q_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                 7.092
_cell_length_b                 12.779
_cell_length_c                 6.712
_cell_angle_alpha               122.17
_cell_angle_beta                58.72
_cell_angle_gamma               132.96
_cell_volume                   364.622
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.12821 0.70183 0.11114
N'2 N -0.28612 0.74534 0.25548
H*3 H -0.47098 0.66092 0.31788
N4 N 0.12487 0.79540 -0.01510
H*5 H 0.27138 0.79375 -0.02714
H*6 H 0.17129 0.89999 0.04244
N7 N -0.17725 0.56504 0.06116
```

H*8 H -0.36932 0.48734 0.12341
H*9 H -0.09577 0.52401 -0.11219
C1+ C -0.12830 -0.25465 0.63841
N2+ N -0.01342 -0.11026 0.67122
N'3+ N -0.19355 -0.07734 0.81582
N'4+ N -0.41565 -0.20082 0.87009
N'5+ N -0.38082 -0.31179 0.76304
O6+ O 0.24197 -0.00721 0.57938
N7+ N 0.00346 -0.33298 0.49163
O8+ O -0.13245 -0.46375 0.48310
O9+ O 0.23989 -0.25966 0.38991
H*10+ H 0.24447 0.08257 0.64559

#END

data_1d_q_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 15.963
_cell_length_b 4.573
_cell_length_c 20.456
_cell_angle_alpha 90.00
_cell_angle_beta 105.26
_cell_angle_gamma 90.00
_cell_volume 1440.61
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.03409 0.57372 -0.10665
N'2 N -0.00130 0.33123 -0.09672
H*3 H 0.03154 0.23641 -0.05219
N4 N 0.00499 0.72153 -0.16807
H*5 H 0.00188 0.94201 -0.16414
H*6 H -0.05023 0.63295 -0.19766
N7 N 0.10178 0.72113 -0.06121
H*8 H 0.13208 0.60295 -0.01996
H*9 H 0.14378 0.82652 -0.08261

```
C1+ C 0.27038 -0.20846 0.64685
N2+ N 0.19339 -0.06861 0.62698
N'3+ N 0.14681 -0.18757 0.56975
N'4+ N 0.19522 -0.39772 0.55510
N'5+ N 0.27171 -0.41519 0.60182
O6+ O 0.16285 0.15798 0.65709
N7+ N 0.33945 -0.14244 0.70720
O8+ O 0.40469 -0.29240 0.71706
O9+ O 0.32542 0.05878 0.74261
H*10+ H 0.10528 0.19454 0.62713

#END

data_1d_q_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                  6.017
_cell_length_b                  10.691
_cell_length_c                  7.378
_cell_angle_alpha                 113.44
_cell_angle_beta                 64.31
_cell_angle_gamma                   119.41
_cell_volume                    362.094
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.67492 0.71868 0.47027
N'2 N 0.81039 0.64116 0.33437
H*3 H 1.00713 0.69396 0.32863
N4 N 0.40820 0.67386 0.48648
H*5 H 0.28551 0.68870 0.63320
H*6 H 0.33642 0.57083 0.39877
N7 N 0.76296 0.84988 0.61498
H*8 H 0.96296 0.89596 0.59028
H*9 H 0.68547 0.92436 0.64670
C1+ C 0.30864 0.19769 -0.06338
N2+ N 0.44097 0.32483 0.05314
N'3+ N 0.27404 0.39129 0.18423
N'4+ N 0.04254 0.30506 0.14734
N'5+ N 0.05847 0.18498 -0.00458
O6+ O 0.70108 0.38407 0.04843
N7+ N 0.42227 0.09347 -0.22491
O8+ O 0.27197 -0.01590 -0.31429
```

O9+ O 0.65961 0.12568 -0.25598
H*10+ H 0.71751 0.47564 0.15580

#END

S31. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

data_1e_q_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 12.351
_cell_length_b 9.338
_cell_length_c 6.945
_cell_angle_alpha 90.00
_cell_angle_beta 104.57
_cell_angle_gamma 90.00
_cell_volume 775.233
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.63221 0.20552 0.77032
N2 N 0.55704 0.31892 0.71823
H*3 H 0.49334 0.29908 0.59695
N'4 N 0.73848 0.23165 0.81657
N5 N 0.58336 0.07174 0.76630
H*6 H 0.50890 0.07179 0.80267
H*7 H 0.63918 -0.00127 0.84236
N8 N 0.80305 0.10406 0.88737
H*9 H 0.82910 0.06342 0.76984
H*10 H 0.87411 0.13997 0.98399
H*11 H 0.59695 0.41198 0.70515
C1+ C 0.32478 -0.22275 0.71668
N2+ N 0.29451 -0.08513 0.73155
N'3+ N 0.18618 -0.07128 0.64572
N'4+ N 0.15117 -0.19950 0.57945
N'5+ N 0.23496 -0.29481 0.62126
O6+ O 0.35816 0.02782 0.81714
N7+ N 0.43662 -0.28092 0.79254
O8+ O 0.44836 -0.40827 0.76529
O9+ O 0.50881 -0.19591 0.87710

```
H*10+ H 0.30545 0.10754 0.79658

#END

data_1e_q_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                 12.465
_cell_length_b                 9.261
_cell_length_c                 7.961
_cell_angle_alpha               90.00
_cell_angle_beta                56.91
_cell_angle_gamma                 90.00
_cell_volume                   769.955
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24850 0.71091 0.24656
N2 N 0.20301 0.82534 0.18842
H*3 H 0.19727 0.80262 0.06888
N'4 N 0.33337 0.73583 0.28876
N5 N 0.19636 0.57750 0.25264
H*6 H 0.10431 0.58116 0.29135
H*7 H 0.21247 0.50524 0.33284
N8 N 0.35864 0.60815 0.36702
H*9 H 0.44000 0.56196 0.25027
H*10 H 0.38432 0.64589 0.46039
H*11 H 0.25290 0.91736 0.16799
C1+ C -0.04208 0.26779 0.23766
N2+ N -0.07904 0.40554 0.24258
N'3+ N -0.14461 0.41216 0.15604
N'4+ N -0.14730 0.27949 0.09920
N'5+ N -0.08479 0.18841 0.14773
O6+ O -0.05739 0.52467 0.31978
N7+ N 0.03172 0.21638 0.31746
O8+ O 0.05637 0.08780 0.29945
O9+ O 0.06228 0.30772 0.39563
H*10+ H -0.09947 0.60203 0.29355

#END
```

```
data_1e_q_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                  11.455
_cell_length_b                  7.519
_cell_length_c                  5.219
_cell_angle_alpha                 65.48
_cell_angle_beta                 89.56
_cell_angle_gamma                   78.04
_cell_volume                    398.545
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.69886 -0.22632 0.56585
N2 N 0.59407 -0.25879 0.47599
H*3 H 0.53857 -0.30548 0.63081
N'4 N 0.80014 -0.29208 0.48863
N5 N 0.68292 -0.12376 0.73543
H*6 H 0.60418 -0.02141 0.69051
H*7 H 0.75619 -0.06963 0.74680
N8 N 0.89677 -0.22577 0.57499
H*9 H 0.93942 -0.34148 0.75751
H*10 H 0.95684 -0.21642 0.42765
H*11 H 0.61200 -0.35051 0.37592
C1+ C 0.77562 0.28137 0.03196
N2+ N 0.77672 0.40524 0.15872
N'3+ N 0.67222 0.43403 0.26371
N'4+ N 0.60838 0.32843 0.20100
N'5+ N 0.67005 0.23290 0.05817
O6+ O 0.86557 0.49317 0.18521
N7+ N 0.87356 0.21365 -0.10838
O8+ O 0.85637 0.10155 -0.21142
O9+ O 0.96456 0.27607 -0.10971
H*10+ H 0.83126 0.57037 0.28945

#END

data_1e_q_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                 10.165
_cell_length_b                 7.941
_cell_length_c                 11.651
_cell_angle_alpha               90.00
_cell_angle_beta               121.86
_cell_angle_gamma                90.00
_cell_volume                   798.781
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.19856 0.56070 0.18941
N2 N 0.07540 0.56527 0.21011
H*3 H 0.03613 0.44975 0.21520
N'4 N 0.19795 0.66147 0.10190
N5 N 0.31265 0.44396 0.26735
H*6 H 0.32893 0.42393 0.35988
H*7 H 0.41165 0.46885 0.26865
N8 N 0.34201 0.65228 0.10472
H*9 H 0.32315 0.57391 0.02779
H*10 H 0.35597 0.76857 0.07579
H*11 H -0.01127 0.64081 0.14181
C1+ C -0.28067 0.54636 0.32409
N2+ N -0.15295 0.63864 0.40542
N'3+ N -0.15385 0.68270 0.51487
N'4+ N -0.28110 0.61761 0.49990
N'5+ N -0.36134 0.53295 0.38314
O6+ O -0.03658 0.68513 0.38705
N7+ N -0.32172 0.47465 0.19445
O8+ O -0.44203 0.39463 0.13483
O9+ O -0.23096 0.50162 0.15726
H*10+ H 0.03281 0.75020 0.46799

#END

data_1e_q_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 17.449
_cell_length_b 7.990
_cell_length_c 5.754
_cell_angle_alpha 90.00
_cell_angle_beta 99.57
_cell_angle_gamma 90.00
_cell_volume 791.044
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.10039 0.89275 0.32947
N2 N -0.16871 0.98571 0.27595
H*3 H -0.16007 1.10599 0.23005
N'4 N -0.09044 0.79710 0.51342
N5 N -0.04832 0.91379 0.17461
H*6 H -0.07345 0.93595 0.00568
H*7 H -0.00805 0.82050 0.19317
N8 N -0.02065 0.69683 0.52651
H*9 H 0.02193 0.75628 0.64057
H*10 H -0.03176 0.59010 0.61173
H*11 H -0.20119 0.97809 0.40634
C1+ C 0.66156 -0.05089 -0.10059
N2+ N 0.64409 0.04598 0.07552
N'3+ N 0.59333 -0.03411 0.18330
N'4+ N 0.58019 -0.17830 0.07329
N'5+ N 0.62153 -0.19177 -0.10241
O6+ O 0.67093 0.20100 0.14436
N7+ N 0.71504 -0.00732 -0.25974
O8+ O 0.72364 -0.11084 -0.40879
O9+ O 0.74655 0.13007 -0.22869
H*10+ H 0.64444 0.22709 0.27645

#END

S32. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

data_1f_q_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                 19.690
_cell_length_b                 8.629
_cell_length_c                 5.406
_cell_angle_alpha               90.00
_cell_angle_beta                82.83
_cell_angle_gamma                 90.00
_cell_volume                   911.324
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.38335 0.25303 0.15031
N'2 N 0.34302 0.15571 0.06020
N3 N 0.44835 0.28247 0.02335
H*4 H 0.48490 0.29207 0.13900
N5 N 0.36895 0.33342 0.37307
N6 N 0.47205 0.19006 -0.18678
N7 N 0.27674 0.14941 0.20759
H*8 H 0.27942 0.07028 0.34708
H*9 H 0.44996 0.08281 -0.16313
H*10 H 0.45285 0.23741 -0.33609
H*11 H 0.24501 0.10116 0.09428
H*12 H 0.39162 0.43892 0.37348
H*13 H 0.31766 0.33671 0.42889
C1+ C 0.14282 0.25078 0.53086
N2+ N 0.13859 0.37593 0.38384
N'3+ N 0.08784 0.35513 0.24715
N'4+ N 0.06157 0.21848 0.31094
N'5+ N 0.09453 0.15173 0.48550
O6+ O 0.17741 0.50672 0.36563
N7+ N 0.19194 0.22930 0.70767
O8+ O 0.18809 0.10833 0.82488
O9+ O 0.23277 0.33544 0.72208
H*10+ H 0.15815 0.56806 0.23975

#END

data_1f_q_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                 10.928
_cell_length_b                 11.894
```

```
_cell_length_c                  7.166
_cell_angle_alpha                90.00
_cell_angle_beta                110.82
_cell_angle_gamma                90.00
_cell_volume                    870.6
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.53322 0.29865 0.13266
N'2 N 0.56115 0.39133 0.23307
N3 N 0.44064 0.22500 0.15795
H*4 H 0.46689 0.14313 0.15973
N5 N 0.58977 0.26135 -0.00158
N6 N 0.39102 0.24695 0.31231
N7 N 0.65130 0.45956 0.17612
H*8 H 0.74426 0.43441 0.25962
H*9 H 0.46162 0.28820 0.42539
H*10 H 0.31645 0.30310 0.25696
H*11 H 0.64260 0.53838 0.22508
H*12 H 0.52942 0.21414 -0.11480
H*13 H 0.63225 0.32602 -0.04915
C1+ C 0.71282 -0.13383 0.29721
N2+ N 0.79595 -0.05032 0.29519
N'3+ N 0.73038 0.04592 0.25334
N'4+ N 0.60854 0.02086 0.23023
N'5+ N 0.59510 -0.08940 0.25648
O6+ O 0.92632 -0.05561 0.32854
N7+ N 0.74724 -0.25176 0.33724
O8+ O 0.65889 -0.31546 0.33268
O9+ O 0.86241 -0.27600 0.37194
H*10+ H 0.94976 0.02210 0.31345

#END

data_1f_q_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                  19.645
_cell_length_b                  6.586
_cell_length_c                  6.702
_cell_angle_alpha                90.00
```

```
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                    867.118
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.16061 0.66676 0.38959
N'2 N 0.21085 0.78743 0.42738
N3 N 0.17286 0.47507 0.30755
H*4 H 0.13841 0.43615 0.20158
N5 N 0.09225 0.71041 0.41960
N6 N 0.23980 0.42664 0.24409
N7 N 0.18853 0.97124 0.52448
H*8 H 0.17507 1.07279 0.41582
H*9 H 0.26349 0.55800 0.20112
H*10 H 0.26566 0.37768 0.36671
H*11 H 0.23100 1.03053 0.58882
H*12 H 0.06335 0.58743 0.45294
H*13 H 0.08640 0.82671 0.51810
C1+ C 0.94872 0.09070 0.51658
N2+ N 0.88160 0.11218 0.47920
N'3+ N 0.85078 -0.06456 0.50892
N'4+ N 0.89887 -0.19199 0.56384
N'5+ N 0.95971 -0.10010 0.56975
O6+ O 0.84674 0.28020 0.42038
N7+ N 0.99972 0.24991 0.50088
O8+ O 1.05811 0.20238 0.54065
O9+ O 0.97903 0.41762 0.44889
H*10+ H 0.79982 0.23287 0.40992

#END

data_1f_q_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                  5.468
_cell_length_b                  11.308
_cell_length_c                  8.941
_cell_angle_alpha               65.50
_cell_angle_beta                83.23
_cell_angle_gamma               107.77
_cell_volume                    459.606
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.41589 0.23024 0.10821
N'2 N -0.23786 0.31060 -0.03887
N3 N -0.41567 0.09917 0.21787
H*4 H -0.60236 0.02225 0.27785
N5 N -0.62078 0.26022 0.17102
N6 N -0.23982 0.04923 0.15622
N7 N -0.25870 0.44505 -0.12784
H*8 H -0.39489 0.43377 -0.19539
H*9 H -0.20953 0.08967 0.02664
H*10 H -0.05877 0.09338 0.17187
H*11 H -0.07924 0.51022 -0.21793
H*12 H -0.67611 0.21814 0.30034
H*13 H -0.57940 0.36554 0.10837
C1+ C 0.33201 0.27543 0.57253
N2+ N 0.17565 0.26887 0.70671
N'3+ N -0.07137 0.17713 0.74446
N'4+ N -0.06454 0.12856 0.63399
N'5+ N 0.18176 0.18745 0.52660
O6+ O 0.24172 0.34004 0.79647
N7+ N 0.61566 0.36388 0.49301
O8+ O 0.72462 0.35588 0.37259
O9+ O 0.71873 0.43846 0.55498
H*10+ H 0.07388 0.30581 0.88229

#END

data_1f_q_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                 19.852
_cell_length_b                 9.022
_cell_length_c                 5.099
_cell_angle_alpha               90.00
_cell_angle_beta                99.15
_cell_angle_gamma                90.00
_cell_volume                   901.634
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.58869 0.18251 0.15857
N'2 N 0.62190 0.20024 0.39582
N3 N 0.52988 0.26573 0.07336
H*4 H 0.49233 0.20571 -0.03616
N5 N 0.60516 0.08282 -0.02870
N6 N 0.50297 0.35495 0.26107
N7 N 0.68354 0.11288 0.44000
H*8 H 0.67122 0.00988 0.50193
H*9 H 0.51502 0.30671 0.44427
H*10 H 0.52903 0.45263 0.27368
H*11 H 0.71298 0.15953 0.60029
H*12 H 0.59189 0.11708 -0.21934
H*13 H 0.65476 0.05038 0.01562
C1+ C 0.16114 -0.21568 0.68592
N2+ N 0.14052 -0.08075 0.59083
N'3+ N 0.09999 -0.09707 0.35923
N'4+ N 0.09612 -0.24074 0.31453
N'5+ N 0.13334 -0.31633 0.51288
O6+ O 0.15591 0.05513 0.69941
N7+ N 0.20602 -0.24458 0.93497
O8+ O 0.21916 -0.37406 0.98866
O9+ O 0.22648 -0.13541 1.06790
H*10+ H 0.13112 0.12329 0.57016

#END
```

S33. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 5-nitrotetrazole 1*N*-oxide (cocrystal form).

```
data_1g_q_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                 7.104
_cell_length_b                 18.462
_cell_length_c                 7.107
_cell_angle_alpha               90.00
_cell_angle_beta                87.71
_cell_angle_gamma                 90.00
_cell_volume                   931.367
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25907 0.42092 -0.54733
N'2 N 0.33245 0.45254 -0.69585
N3 N 0.36365 0.40209 -0.84921
N4 N 0.20424 0.34842 -0.54458
N5 N 0.16835 0.31630 -0.36562
N6 N 0.22963 0.45953 -0.38233
N7 N 0.23516 0.53600 -0.38726
H*8 H 0.45010 0.42844 -0.94387
H*9 H 0.23921 0.39519 -0.91498
H*10 H 0.28304 0.31953 -0.64145
H*11 H 0.06808 0.27763 -0.37883
H*12 H 0.28690 0.29302 -0.31634
H*13 H 0.13218 0.43874 -0.28991
H*14 H 0.37360 0.55066 -0.39551
H*15 H 0.18225 0.55284 -0.51188
C1+ C 0.76045 0.19125 0.45676
N2+ N 0.75075 0.12319 0.38855
N'3+ N 0.90521 0.08742 0.43166
N'4+ N 1.00756 0.13346 0.52522
N'5+ N 0.92153 0.19786 0.54263
O6+ O 0.61214 0.09164 0.29056
N7+ N 0.61833 0.24723 0.43857
O8+ O 0.65133 0.30574 0.50942
O9+ O 0.47816 0.23015 0.35330
H*10+ H 0.65845 0.04255 0.26774

#END

data_1g_q_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                 6.489
_cell_length_b                 21.281
_cell_length_c                 6.786
_cell_angle_alpha               90.00
_cell_angle_beta                89.65
_cell_angle_gamma                 90.00
_cell_volume                   937.078
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.19895 -0.33254 0.78913
N'2 N -0.31375 -0.28589 0.73415
N3 N -0.50371 -0.30736 0.64717
N4 N -0.26200 -0.39506 0.77865
N5 N -0.10740 -0.44163 0.79862
N6 N -0.00519 -0.32139 0.86471
N7 N 0.04739 -0.26014 0.92701
H*8 H -0.56335 -0.26903 0.57865
H*9 H -0.60539 -0.31787 0.75844
H*10 H -0.36646 -0.40074 0.66830
H*11 H -0.17235 -0.48017 0.86174
H*12 H -0.04651 -0.45379 0.66504
H*13 H 0.05373 -0.35615 0.94883
H*14 H 0.08086 -0.23480 0.80340
H*15 H -0.08193 -0.23937 0.98475
C1+ C 0.54042 0.56762 0.23778
N2+ N 0.57942 0.62983 0.22709
N'3+ N 0.41815 0.65858 0.14845
N'4+ N 0.28263 0.61413 0.11185
N'5+ N 0.35420 0.55763 0.16554
O6+ O 0.75029 0.66197 0.28351
N7+ N 0.67934 0.52017 0.31527
O8+ O 0.61772 0.46608 0.31318
O9+ O 0.84604 0.53917 0.37562
H*10+ H 0.71769 0.70551 0.25141

#END

data_1g_q_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                 5.470
_cell_length_b                 18.941
_cell_length_c                 9.350
_cell_angle_alpha               90.00
_cell_angle_beta                77.29
_cell_angle_gamma                 90.00
_cell_volume                   944.99
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.69437 -0.17123 -0.26866
N'2 N 0.47886 -0.14691 -0.19973
N3 N 0.42981 -0.16344 -0.04528
N4 N 0.86304 -0.20404 -0.19794
N5 N 1.06199 -0.24256 -0.28676
N6 N 0.76759 -0.16440 -0.41909
N7 N 0.63954 -0.11655 -0.49257
H*8 H 0.24397 -0.15382 -0.00738
H*9 H 0.52050 -0.12708 0.00549
H*10 H 0.76960 -0.22721 -0.10308
H*11 H 1.21209 -0.24027 -0.23945
H*12 H 1.01373 -0.29409 -0.29610
H*13 H 0.95408 -0.16743 -0.46112
H*14 H 0.47603 -0.14027 -0.50106
H*15 H 0.58584 -0.07395 -0.42554
C1+ C 0.98896 -0.06067 0.23760
N2+ N 0.85724 -0.00184 0.22316
N'3+ N 0.70725 -0.01514 0.13250
N'4+ N 0.74787 -0.08149 0.09240
N'5+ N 0.92070 -0.11075 0.15563
O6+ O 0.86407 0.06259 0.28629
N7+ N 1.17326 -0.06745 0.32761
O8+ O 1.27403 -0.12485 0.32719
O9+ O 1.20994 -0.01452 0.39570
H*10+ H 0.74209 0.09024 0.24812

#END

data_1g_q_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                14.203
_cell_length_b                7.399
_cell_length_c                9.099
_cell_angle_alpha              90.00
_cell_angle_beta               103.14
_cell_angle_gamma               90.00
_cell_volume                  931.16
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.33019 0.13355 -0.54583
N'2 N 0.24617 0.08514 -0.52600
N3 N 0.17334 0.09014 -0.66550
N4 N 0.34774 0.17088 -0.68738
N5 N 0.43496 0.26220 -0.69065
N6 N 0.40787 0.14793 -0.42357
N7 N 0.40230 0.06843 -0.28463
H*8 H 0.10915 0.08240 -0.63422
H*9 H 0.17812 -0.02663 -0.72386
H*10 H 0.28605 0.21512 -0.75914
H*11 H 0.45677 0.22201 -0.78435
H*12 H 0.42543 0.39889 -0.69418
H*13 H 0.47386 0.14044 -0.44751
H*14 H 0.36181 0.15266 -0.23516
H*15 H 0.36229 -0.04764 -0.30685
C1+ C 0.86377 -0.26702 0.07709
N2+ N 0.82000 -0.22244 0.18907
N'3+ N 0.73527 -0.30613 0.16643
N'4+ N 0.72783 -0.40060 0.04174
N'5+ N 0.80608 -0.37885 -0.01558
O6+ O 0.85158 -0.11174 0.30949
N7+ N 0.95783 -0.20291 0.06165
O8+ O 0.98593 -0.25778 -0.04722
O9+ O 1.00013 -0.09925 0.16010
H*10+ H 0.79939 -0.11538 0.36302

#END

data_1g_q_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                 19.558
_cell_length_b                 9.001
_cell_length_c                 5.527
_cell_angle_alpha               90.00
_cell_angle_beta               103.54
_cell_angle_gamma                90.00
_cell_volume                   945.939
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.08569 -0.17732 -0.17488
N'2 N -0.12670 -0.20364 -0.39147
N3 N -0.18866 -0.11092 -0.43729
N4 N -0.09824 -0.06458 -0.01785
N5 N -0.05955 -0.06969 0.23322
N6 N -0.02581 -0.26166 -0.09132
N7 N -0.00017 -0.34999 -0.26208
H*8 H -0.22228 -0.15741 -0.58648
H*9 H -0.17588 -0.00913 -0.49701
H*10 H -0.15082 -0.04316 -0.04983
H*11 H -0.05218 0.03614 0.29777
H*12 H -0.08583 -0.12810 0.34118
H*13 H 0.01205 -0.21442 0.04285
H*14 H -0.03078 -0.44290 -0.29426
H*15 H -0.00997 -0.29561 -0.42945
C1+ C 0.66084 -0.21125 0.69313
N2+ N 0.64227 -0.07568 0.59525
N'3+ N 0.60382 -0.09164 0.36470
N'4+ N 0.59916 -0.23571 0.32340
N'5+ N 0.63385 -0.31194 0.52289
O6+ O 0.65778 0.06046 0.70041
N7+ N 0.70311 -0.24070 0.94210
O8+ O 0.71464 -0.37073 0.99858
O9+ O 0.72322 -0.13141 1.07215
H*10+ H 0.63480 0.12910 0.56998

#END
```

S34. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

```
data_2a_q_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                 9.586
_cell_length_b                 16.903
_cell_length_c                 7.606
_cell_angle_alpha               90.00
_cell_angle_beta                45.01
_cell_angle_gamma                 90.00
```

```
_cell_volume                    871.602
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.29299 -0.42606 0.55341
H*2 H 0.25476 -0.45743 0.47824
H*3 H 0.19809 -0.37945 0.64601
H*4 H 0.26536 -0.46146 0.68366
C1+ C -0.24437 0.57824 -0.19210
N'2+ N -0.25896 0.50193 0.05361
N'3+ N -0.25087 0.45875 -0.09513
N'4+ N -0.24116 0.50422 -0.25050
N5+ N -0.25575 0.57677 -0.00461
C6+ C -0.23995 0.65080 -0.30511
N7+ N -0.03720 0.69447 -0.47997
O8+ O 0.00359 0.73494 -0.64237
O9+ O 0.05665 0.68445 -0.42910
N10+ N -0.28437 0.63028 -0.46040
O11+ O -0.15426 0.59414 -0.64979
O12+ O -0.44322 0.65143 -0.37562
N13+ N -0.39877 0.71164 -0.10130
O14+ O -0.54650 0.68228 0.09395
O15+ O -0.36262 0.78099 -0.15583
O16+ O -0.25897 0.63944 0.11011
H*17+ H -0.39498 0.64356 0.27165

#END

data_2a_q_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                  7.579
_cell_length_b                  6.688
_cell_length_c                  9.236
_cell_angle_alpha                90.89
_cell_angle_beta                108.47
_cell_angle_gamma                92.57
_cell_volume                    443.378
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

```
_atom_site_fract_z
N1 N 0.30718 0.76425 -0.12932
H*2 H 0.44158 0.74728 -0.06381
H*3 H 0.27497 0.65569 -0.21357
H*4 H 0.22592 0.73318 -0.06238
C1+ C 0.00900 0.74764 0.16115
N'2+ N -0.27374 0.78566 0.00727
N'3+ N -0.16062 0.76402 -0.07186
N'4+ N 0.01585 0.73956 0.02007
N5+ N -0.16915 0.77644 0.15318
C6+ C 0.16605 0.73199 0.30428
N7+ N 0.16307 0.52714 0.38240
O8+ O 0.31145 0.47329 0.46311
O9+ O 0.00904 0.44539 0.35620
N10+ N 0.35450 0.75810 0.27203
O11+ O 0.38810 0.61961 0.20082
O12+ O 0.44584 0.91308 0.31918
N13+ N 0.16358 0.89824 0.42428
O14+ O 0.09903 1.05410 0.37001
O15+ O 0.22708 0.85897 0.55762
O16+ O -0.24018 0.79012 0.27064
H*17+ H -0.26076 0.93159 0.28130

#END

data_2a_q_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                 17.545
_cell_length_b                 9.263
_cell_length_c                 10.901
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1771.62
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

```
_atom_site_fract_z
N1 N 0.14821 0.59157 -0.44508
H*2 H 0.16948 0.53172 -0.37450
H*3 H 0.14941 0.52765 -0.52114
H*4 H 0.09230 0.61078 -0.42565
C1+ C 0.30846 0.81873 -0.15853
N'2+ N 0.19195 0.75084 -0.20284
N'3+ N 0.21358 0.85203 -0.27804
N'4+ N 0.28567 0.89635 -0.25332
N5+ N 0.25070 0.72945 -0.12736
C6+ C 0.38285 0.82728 -0.09473
N7+ N 0.43644 0.69726 -0.12398
O8+ O 0.50417 0.71874 -0.11398
O9+ O 0.40366 0.58600 -0.15103
N10+ N 0.42535 0.96756 -0.13179
O11+ O 0.44859 0.96842 -0.23628
O12+ O 0.42996 1.06084 -0.05390
N13+ N 0.37216 0.82989 0.04756
O14+ O 0.31335 0.88637 0.08253
O15+ O 0.42273 0.77843 0.10901
O16+ O 0.24973 0.62899 -0.03656
H*17+ H 0.21833 0.67013 0.02835

#END

data_2a_q_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                 7.489
_cell_length_b                 9.633
_cell_length_c                 6.558
_cell_angle_alpha               76.73
_cell_angle_beta               102.80
_cell_angle_gamma               81.65
_cell_volume                   439.343
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.29923 0.47246 0.20186
H*2 H 0.28009 0.49181 0.03828
H*3 H 0.20664 0.41037 0.24246
H*4 H 0.42987 0.40956 0.27356
C1+ C 0.00727 0.25729 0.56574
```

N'2+ N -0.28837 0.34675 0.39419
N'3+ N -0.18335 0.39022 0.26876
N'4+ N 0.00086 0.33638 0.36994
N5+ N -0.17073 0.26399 0.58068
C6+ C 0.17653 0.17681 0.74154
N7+ N 0.20940 0.00832 0.77636
O8+ O 0.36917 -0.05881 0.85442
O9+ O 0.06810 -0.03807 0.72550
N10+ N 0.35302 0.22749 0.69014
O11+ O 0.39743 0.18986 0.54146
O12+ O 0.42548 0.29980 0.80081
N13+ N 0.16352 0.20483 0.96375
O14+ O 0.07405 0.32428 0.95018
O15+ O 0.24403 0.10808 1.12615
O16+ O -0.22987 0.19671 0.75187
H*17+ H -0.26810 0.27300 0.81790

#END

data_2a_q_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 7.646
_cell_length_b 6.532
_cell_length_c 8.671
_cell_angle_alpha 93.91
_cell_angle_beta 96.96
_cell_angle_gamma 86.44
_cell_volume 428.236
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.15677 -0.27067 0.78457
H*2 H -0.10379 -0.14919 0.85001
H*3 H -0.29002 -0.24132 0.77007
H*4 H -0.11495 -0.26946 0.67744
C1+ C 0.08830 0.23532 0.67287
N'2+ N -0.19989 0.22721 0.65158
N'3+ N -0.14972 0.25359 0.51644
N'4+ N 0.02836 0.25879 0.52541
N5+ N -0.05226 0.21634 0.75048
C6+ C 0.27447 0.23313 0.74412
N7+ N 0.35195 0.01404 0.78477

O8+ O 0.51025 -0.01511 0.78932
O9+ O 0.24357 -0.10344 0.81162
N10+ N 0.39212 0.31749 0.63182
O11+ O 0.41206 0.20516 0.51775
O12+ O 0.44909 0.48550 0.66857
N13+ N 0.29464 0.37116 0.89898
O14+ O 0.18908 0.51838 0.90331
O15+ O 0.41244 0.32200 0.99778
O16+ O -0.05176 0.18566 0.90397
H*17+ H -0.09137 0.31721 0.95147

#END

S35. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

data_2b_q_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 5.988
_cell_length_b 9.667
_cell_length_c 15.560
_cell_angle_alpha 90.00
_cell_angle_beta 90.55
_cell_angle_gamma 90.00
_cell_volume 900.665
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 1.01957 0.85140 0.32956
H*2 H 1.04873 0.92913 0.37277
H*3 H 0.89253 0.88588 0.29079
O4 O 0.91734 0.74378 0.38030
H*5 H 1.01263 0.66521 0.36969
C1+ C 0.37325 0.18458 -0.12723
N'2+ N 0.23058 0.03000 -0.04048
N'3+ N 0.17821 0.00004 -0.11971
N'4+ N 0.26456 0.09365 -0.17521
N5+ N 0.35185 0.14551 -0.04432
C6+ C 0.49466 0.30897 -0.15687
N7+ N 0.75381 0.29252 -0.15225

```
O8+ O 0.86087 0.36276 -0.20128
O9+ O 0.82085 0.21228 -0.09757
N10+ N 0.43008 0.34246 -0.25143
O11+ O 0.50089 0.26085 -0.30344
O12+ O 0.31503 0.44429 -0.26302
N13+ N 0.43534 0.43813 -0.10120
O14+ O 0.24711 0.43774 -0.07220
O15+ O 0.57774 0.52603 -0.09305
O16+ O 0.44033 0.20759 0.02656
H*17+ H 0.31602 0.25468 0.05398

#END

data_2b_q_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                  14.378
_cell_length_b                  10.295
_cell_length_c                  7.611
_cell_angle_alpha                97.98
_cell_angle_beta                 130.50
_cell_angle_gamma                122.81
_cell_volume                    461.255
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.70520 0.15914 -0.00920
H*2 H 0.72485 0.13797 -0.11192
H*3 H 0.82836 0.22833 0.23019
O4 O 0.50029 -0.08499 -0.24266
H*5 H 0.40955 -0.09161 -0.32440
C1+ C 0.13559 0.39099 -0.10174
N'2+ N -0.01022 0.33279 -0.04571
N'3+ N -0.13898 0.24873 -0.35108
N'4+ N -0.05376 0.28132 -0.39486
N5+ N 0.16250 0.42305 0.11329
C6+ C 0.29481 0.47032 -0.01422
N7+ N 0.28447 0.30812 -0.05054
O8+ O 0.34229 0.30254 -0.11204
O9+ O 0.22390 0.20849 -0.00335
N10+ N 0.24437 0.46759 -0.26830
O11+ O 0.07128 0.26793 -0.57763
O12+ O 0.38008 0.66266 -0.13349
```

```
N13+ N 0.54307 0.73316 0.38178
O14+ O 0.56572 0.86291 0.49589
O15+ O 0.68780 0.78407 0.53457
O16+ O 0.33182 0.52434 0.43850
H*17+ H 0.42598 0.68341 0.61659

#END

data_2b_q_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                 10.469
_cell_length_b                 11.989
_cell_length_c                 7.231
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   907.583
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.41966 0.15987 0.69168
H*2 H 0.39013 0.12661 0.81462
H*3 H 0.51651 0.16833 0.70284
O4 O 0.37291 0.27327 0.69724
H*5 H 0.32334 0.27842 0.58503
C1+ C -0.11522 0.09017 0.75996
N'2+ N -0.28678 0.13765 0.91500
N'3+ N -0.29922 0.16642 0.74233
N'4+ N -0.19463 0.13791 0.64214
N5+ N -0.17189 0.09026 0.92789
C6+ C 0.01382 0.04562 0.72011
N7+ N 0.01871 -0.08448 0.71636
O8+ O 0.10235 -0.12618 0.62392
O9+ O -0.06129 -0.13026 0.81190
N10+ N 0.06130 0.08829 0.52952
O11+ O 0.00571 0.04867 0.39838
O12+ O 0.14671 0.15677 0.53196
N13+ N 0.11239 0.08431 0.86915
O14+ O 0.09002 0.17502 0.93775
O15+ O 0.20122 0.02265 0.90052
```

O16+ O -0.12558 0.04770 1.08863
H*17+ H -0.09959 0.11198 1.16198

#END

data_2b_q_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 15.017
_cell_length_b 9.773
_cell_length_c 6.470
_cell_angle_alpha 90.00
_cell_angle_beta 89.43
_cell_angle_gamma 90.00
_cell_volume 949.498
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.44948 0.62943 0.40687
H*2 H -0.41112 0.63627 0.27588
H*3 H -0.42557 0.54701 0.48620
O4 O -0.53497 0.58370 0.33280
H*5 H -0.57506 0.65274 0.38584
C1+ C 0.14645 -0.29432 -0.17956
N'2+ N 0.00045 -0.29248 -0.17787
N'3+ N 0.02947 -0.40562 -0.26064
N'4+ N 0.11978 -0.41025 -0.26362
N5+ N 0.07300 -0.22179 -0.12725
C6+ C 0.23939 -0.24830 -0.14933
N7+ N 0.26954 -0.25610 0.08054
O8+ O 0.34859 -0.26871 0.10938
O9+ O 0.20960 -0.24504 0.20732
N10+ N 0.30439 -0.33752 -0.27969
O11+ O 0.31239 -0.45371 -0.21813
O12+ O 0.33898 -0.28285 -0.42862
N13+ N 0.25192 -0.09643 -0.21925
O14+ O 0.20394 -0.06061 -0.35997
O15+ O 0.30789 -0.02999 -0.13106
O16+ O 0.06915 -0.09764 -0.03309
H*17+ H 0.05318 -0.03289 -0.14107

```
#END

data_2b_q_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                 7.526
_cell_length_b                 12.523
_cell_length_c                 6.838
_cell_angle_alpha               46.05
_cell_angle_beta                92.91
_cell_angle_gamma                81.84
_cell_volume                   449.096
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.10583 0.60022 -0.24857
H*2 H -0.03144 0.61071 -0.24920
H*3 H 0.12423 0.60126 -0.39692
O4 O 0.18932 0.44376 0.01013
H*5 H 0.27671 0.45550 0.09865
C1+ C 0.53565 0.25295 -0.15649
N'2+ N 0.25250 0.34571 -0.38887
N'3+ N 0.36602 0.38591 -0.55447
N'4+ N 0.54286 0.32993 -0.41684
N5+ N 0.35693 0.26299 -0.13959
C6+ C 0.69221 0.17157 0.07768
N7+ N 0.73386 -0.00613 0.28609
O8+ O 0.88972 -0.07667 0.41840
O9+ O 0.60203 -0.05512 0.29778
N10+ N 0.86881 0.22103 -0.03296
O11+ O 0.93045 0.17534 -0.12985
O12+ O 0.92443 0.30053 -0.01413
N13+ N 0.65517 0.20923 0.24929
O14+ O 0.55884 0.33651 0.11549
O15+ O 0.72615 0.11136 0.49388
O16+ O 0.28618 0.19856 0.08988
H*17+ H 0.23603 0.28220 0.07075

#END
```

S36. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

```
data_2c_q_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                 6.282
_cell_length_b                 17.126
_cell_length_c                 9.205
_cell_angle_alpha               90.00
_cell_angle_beta                78.09
_cell_angle_gamma                90.00
_cell_volume                   969.006
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.31766 0.78924 -0.29403
H*2 H -0.20888 0.80676 -0.38644
H*3 H -0.44363 0.76264 -0.32801
N4 N -0.40498 0.85403 -0.20154
H*5 H -0.30564 0.86357 -0.12902
H*6 H -0.40853 0.90395 -0.26145
C1+ C 0.01783 0.14557 0.70891
N'2+ N -0.23554 0.23515 0.76276
N'3+ N -0.11661 0.24829 0.63157
N'4+ N 0.04177 0.19368 0.59454
N5+ N -0.15254 0.17122 0.81249
C6+ C 0.15276 0.07645 0.72500
N7+ N 0.03616 -0.00257 0.70864
O8+ O 0.15226 -0.05804 0.66752
O9+ O -0.16138 -0.00010 0.74312
N10+ N 0.36715 0.07809 0.60585
O11+ O 0.34380 0.06614 0.48054
O12+ O 0.53263 0.09187 0.64980
N13+ N 0.21521 0.07506 0.88074
O14+ O 0.23345 0.13917 0.93415
O15+ O 0.24224 0.01175 0.93228
O16+ O -0.23719 0.13862 0.94654
H*17+ H -0.18982 0.17194 1.01961

#END

data_2c_q_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                   8.030
_cell_length_b                   19.601
_cell_length_c                   5.930
_cell_angle_alpha                 90.00
_cell_angle_beta                  84.40
_cell_angle_gamma                    90.00
_cell_volume                     928.904
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.75067 0.67474 -0.83977
H*2 H 0.68224 0.64351 -0.93290
H*3 H 0.80198 0.64545 -0.72306
N4 N 0.64865 0.72563 -0.71906
H*5 H 0.64502 0.76695 -0.82211
H*6 H 0.52870 0.70928 -0.67988
C1+ C 0.09163 0.60904 -0.25054
N'2+ N -0.07596 0.68823 -0.35945
N'3+ N -0.13375 0.62816 -0.40383
N'4+ N -0.03302 0.57787 -0.33787
N5+ N 0.06530 0.67695 -0.26433
C6+ C 0.23694 0.57688 -0.15691
N7+ N 0.22665 0.57984 0.10712
O8+ O 0.30170 0.53601 0.19919
O9+ O 0.14661 0.62759 0.19215
N10+ N 0.25088 0.50074 -0.22799
O11+ O 0.14209 0.46459 -0.13711
O12+ O 0.36626 0.48583 -0.36693
N13+ N 0.40401 0.61277 -0.24731
O14+ O 0.40496 0.63688 -0.43675
O15+ O 0.51592 0.61256 -0.12477
O16+ O 0.16058 0.72814 -0.19099
H*17+ H 0.22004 0.74751 -0.32721

#END

data_2c_q_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                 8.302
_cell_length_b                 18.142
_cell_length_c                 10.543
_cell_angle_alpha               90.00
_cell_angle_beta                37.77
_cell_angle_gamma                 90.00
_cell_volume                   972.598
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.34183 0.64310 -0.04501
H*2 H 0.49479 0.60709 -0.13140
H*3 H 0.26998 0.65314 0.08804
N4 N 0.13124 0.61304 0.01140
H*5 H 0.16657 0.62630 -0.10273
H*6 H 0.12259 0.55699 0.02304
C1+ C 0.58275 0.14475 0.03370
N'2+ N 0.31194 0.23108 0.13818
N'3+ N 0.44656 0.20612 -0.04146
N'4+ N 0.61596 0.15235 -0.11052
N5+ N 0.39607 0.19332 0.18646
C6+ C 0.72448 0.09371 0.03121
N7+ N 0.55338 0.02692 0.18128
O8+ O 0.67062 -0.02849 0.13791
O9+ O 0.31792 0.03870 0.33031
N10+ N 0.97245 0.06251 -0.19006
O11+ O 0.92601 0.01963 -0.24612
O12+ O 1.18330 0.08469 -0.28309
N13+ N 0.81718 0.13401 0.09662
O14+ O 0.86761 0.19916 0.05150
O15+ O 0.83367 0.09739 0.18189
O16+ O 0.29667 0.20349 0.36668
H*17+ H 0.37397 0.24934 0.34899

#END

data_2c_q_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                 7.723
_cell_length_b                 8.693
_cell_length_c                 14.446
_cell_angle_alpha               90.00
_cell_angle_beta                103.25
_cell_angle_gamma                90.00
_cell_volume                   944.029
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.38532 0.93961 -0.41819
H*2 H 0.36992 0.85643 -0.46924
H*3 H 0.49855 0.91591 -0.36855
N4 N 0.24079 0.94089 -0.37083
H*5 H 0.14555 1.01252 -0.40780
H*6 H 0.18512 0.83466 -0.36988
C1+ C 0.15688 0.31314 0.64751
N'2+ N 0.01522 0.28760 0.76193
N'3+ N -0.06369 0.20697 0.68838
N'4+ N 0.02104 0.21991 0.61620
N5+ N 0.15297 0.35500 0.73710
C6+ C 0.28963 0.36631 0.59510
N7+ N 0.47530 0.28838 0.62969
O8+ O 0.56750 0.28079 0.57250
O9+ O 0.50918 0.24670 0.71228
N10+ N 0.22369 0.33190 0.48736
O11+ O 0.22287 0.19684 0.46707
O12+ O 0.17859 0.44197 0.43576
N13+ N 0.32064 0.54359 0.60651
O14+ O 0.19167 0.61694 0.61635
O15+ O 0.46626 0.59132 0.60329
O16+ O 0.26943 0.44752 0.79692
H*17+ H 0.20746 0.54492 0.79793

#END

data_2c_q_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                 6.436
_cell_length_b                 10.791
_cell_length_c                 7.796
_cell_angle_alpha               112.97
_cell_angle_beta                91.64
_cell_angle_gamma                 74.66
_cell_volume                   479.047
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.12132 0.44972 0.21381
H*2 H 0.20487 0.40629 0.29911
H*3 H -0.03831 0.46120 0.23868
N4 N 0.18176 0.36153 0.01953
H*5 H 0.30741 0.38722 -0.02122
H*6 H 0.23251 0.25809 -0.00304
C1+ C -0.39069 0.27386 0.48121
N'2+ N -0.51075 0.40558 0.77367
N'3+ N -0.65214 0.43662 0.66363
N'4+ N -0.58302 0.35658 0.48121
N5+ N -0.34615 0.30429 0.66120
C6+ C -0.24506 0.16783 0.31634
N7+ N -0.23648 0.01432 0.28385
O8+ O -0.18936 -0.07222 0.12523
O9+ O -0.27334 -0.00228 0.42441
N10+ N -0.31967 0.18991 0.13680
O11+ O -0.48654 0.16073 0.08681
O12+ O -0.20620 0.23496 0.06778
N13+ N -0.00786 0.17923 0.33716
O14+ O 0.00807 0.29684 0.42729
O15+ O 0.13564 0.07273 0.26125
O16+ O -0.16752 0.24291 0.72648
H*17+ H -0.08254 0.31031 0.76753

#END
```

S37. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

```
data_2d_q_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                 12.562
_cell_length_b                 13.889
_cell_length_c                 6.062
_cell_angle_alpha               90.00
_cell_angle_beta                102.91
_cell_angle_gamma                 90.00
_cell_volume                   1030.92
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.13283 0.45013 -0.45368
N'2 N 0.10317 0.38600 -0.32696
H*3 H 0.05088 0.33739 -0.42026
N4 N 0.19451 0.52920 -0.35766
H*5 H 0.25454 0.54913 -0.43556
H*6 H 0.22074 0.52245 -0.18776
N7 N 0.11118 0.45137 -0.69028
H*8 H 0.05500 0.40258 -0.76597
H*9 H 0.09873 0.51760 -0.76170
C1+ C 0.37821 0.25537 0.14117
N'2+ N 0.26321 0.16164 -0.08734
N'3+ N 0.36255 0.13067 -0.06986
N'4+ N 0.43592 0.18703 0.07112
N5+ N 0.27197 0.23981 0.04321
C6+ C 0.42009 0.33618 0.29566
N7+ N 0.39829 0.32312 0.53747
O8+ O 0.46022 0.36403 0.69019
O9+ O 0.31863 0.27450 0.54505
N10+ N 0.54520 0.34708 0.32131
O11+ O 0.59879 0.28303 0.42721
O12+ O 0.57561 0.41689 0.23170
N13+ N 0.36569 0.43348 0.20214
O14+ O 0.33987 0.43883 -0.00346
O15+ O 0.35570 0.49402 0.33951
O16+ O 0.18404 0.29150 0.07078
H*17+ H 0.16103 0.32886 -0.06772

#END

data_2d_q_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 6.113
_cell_length_b 9.300
_cell_length_c 9.752
_cell_angle_alpha 90.97
_cell_angle_beta 72.91
_cell_angle_gamma 87.92
_cell_volume 529.359
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.68554 0.78237 0.69227
N'2 N 0.48907 0.72579 0.73352
H*3 H 0.36588 0.78905 0.70983
N4 N 0.87166 0.72103 0.72870
H*5 H 1.02296 0.72012 0.64991
H*6 H 0.83675 0.62401 0.77395
N7 N 0.74302 0.90438 0.60940
H*8 H 0.60718 0.96240 0.59712
H*9 H 0.85947 0.96644 0.63457
C1+ C 0.53901 -0.26612 0.29022
N'2+ N 0.25682 -0.40406 0.39223
N'3+ N 0.26397 -0.29832 0.47978
N'4+ N 0.43669 -0.21047 0.41974
N5+ N 0.42854 -0.38540 0.27350
C6+ C 0.74070 -0.21162 0.18170
N7+ N 0.67898 -0.13768 0.05461
O8+ O 0.80778 -0.04839 -0.00788
O9+ O 0.50886 -0.18120 0.02972
N10+ N 0.86018 -0.09993 0.25201
O11+ O 0.75266 0.01331 0.28709
O12+ O 1.04451 -0.13780 0.26579
N13+ N 0.92055 -0.33630 0.11442
O14+ O 0.92585 -0.43466 0.19444
O15+ O 1.03814 -0.32326 -0.00797
O16+ O 0.47328 -0.47465 0.15589
H*17+ H 0.54741 -0.56113 0.17990

#END

data_2d_q_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                 10.347
_cell_length_b                 12.141
_cell_length_c                 8.992
_cell_angle_alpha               90.00
_cell_angle_beta                74.22
_cell_angle_gamma                 90.00
_cell_volume                   1087.03
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.10782 0.66521 0.42318
N'2 N 0.16042 0.65600 0.27686
H*3 H 0.26159 0.66920 0.24829
N4 N -0.03127 0.66236 0.48412
H*5 H -0.06407 0.61995 0.58444
H*6 H -0.07883 0.64062 0.40381
N7 N 0.17518 0.67763 0.53760
H*8 H 0.27424 0.69462 0.49673
H*9 H 0.12830 0.72632 0.62773
C1+ C 0.29442 0.08833 0.46198
N'2+ N 0.15372 0.13354 0.68334
N'3+ N 0.25196 0.20420 0.64772
N'4+ N 0.34087 0.17876 0.51085
N5+ N 0.17942 0.06044 0.56834
C6+ C 0.35605 0.02597 0.31868
N7+ N 0.28084 0.04153 0.19138
O8+ O 0.34658 0.02844 0.05906
O9+ O 0.16187 0.06269 0.24017
N10+ N 0.50381 0.06285 0.24935
O11+ O 0.51615 0.15459 0.19477
O12+ O 0.59006 -0.00252 0.25862
N13+ N 0.35700 -0.10038 0.35144
O14+ O 0.36599 -0.12432 0.47979
O15+ O 0.35072 -0.16181 0.24775
O16+ O 0.09681 -0.02575 0.56377
H*17+ H 0.11299 -0.07935 0.63733

#END

data_2d_q_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 18.749
_cell_length_b 5.880
_cell_length_c 9.761
_cell_angle_alpha 90.00
_cell_angle_beta 73.43
_cell_angle_gamma 90.00
_cell_volume 1031.4
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.08601 -0.02768 0.35537
N'2 N 0.06549 -0.21637 0.31207
H*3 H 0.10205 -0.34408 0.31389
N4 N 0.04821 0.17327 0.34603
H*5 H 0.04055 0.27903 0.43101
H*6 H 0.00092 0.14441 0.31816
N7 N 0.14451 0.00620 0.41565
H*8 H 0.17910 -0.12850 0.40681
H*9 H 0.17205 0.15566 0.39005
C1+ C 0.64942 0.20289 -0.27061
N'2+ N 0.59647 -0.03059 -0.38709
N'3+ N 0.66507 0.00679 -0.46114
N'4+ N 0.69959 0.15046 -0.39179
N5+ N 0.58594 0.09180 -0.26795
C6+ C 0.65894 0.35765 -0.15741
N7+ N 0.66525 0.22970 -0.02123
O8+ O 0.69852 0.32669 0.05106
O9+ O 0.63395 0.04634 -0.00054
N10+ N 0.73037 0.50294 -0.21442
O11+ O 0.78780 0.39728 -0.23441
O12+ O 0.72132 0.70335 -0.23429
N13+ N 0.59169 0.52466 -0.10735
O14+ O 0.56215 0.57518 -0.19927
O15+ O 0.57599 0.58989 0.01516
O16+ O 0.52051 0.09305 -0.16234
H*17+ H 0.48705 0.18843 -0.19757

#END

data_2d_q_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 23.988
_cell_length_b 5.914
_cell_length_c 16.260
_cell_angle_alpha 90.00
_cell_angle_beta 77.32
_cell_angle_gamma 90.00
_cell_volume 2250.47
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.56682 -0.06144 0.11864
N'2 N 0.53794 -0.18206 0.07710
H*3 H 0.50434 -0.09353 0.06425
N4 N 0.61065 -0.15849 0.15056
H*5 H 0.64596 -0.06091 0.14572
H*6 H 0.61967 -0.31803 0.12900
N7 N 0.56029 0.16946 0.13693
H*8 H 0.52438 0.23856 0.12473
H*9 H 0.56732 0.21588 0.19382
C1+ C 0.13368 0.97235 -0.13668
N'2+ N 0.05070 1.11975 -0.14211
N'3+ N 0.08742 1.15862 -0.21246
N'4+ N 0.13930 1.06894 -0.21129
N5+ N 0.07918 1.00411 -0.09409
C6+ C 0.17838 0.85320 -0.10343
N7+ N 0.17083 0.59097 -0.10082
O8+ O 0.21362 0.47983 -0.10423
O9+ O 0.12183 0.52638 -0.09341
N10+ N 0.23836 0.90617 -0.15870
O11+ O 0.24756 0.82136 -0.22808
O12+ O 0.26898 1.02725 -0.12747
N13+ N 0.17821 0.93003 -0.01142
O14+ O 0.16306 1.12464 0.00471
O15+ O 0.19358 0.79308 0.03423
O16+ O 0.05435 0.92957 -0.01554
H*17+ H 0.05085 1.06243 0.02067

#END

S38. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

```
data_2e_q_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                  12.716
_cell_length_b                  6.834
_cell_length_c                  13.450
_cell_angle_alpha                90.00
_cell_angle_beta                 77.39
_cell_angle_gamma                   90.00
_cell_volume                    1140.63
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.12131 0.13199 -0.40293
N2 N 0.14398 0.33115 -0.39892
H*3 H 0.09429 0.40315 -0.34123
N'4 N 0.12006 0.05238 -0.48992
N5 N 0.10144 0.03690 -0.30980
H*6 H 0.14313 0.09071 -0.25968
H*7 H 0.10708 -0.11078 -0.31920
N8 N 0.10702 -0.15798 -0.48105
H*9 H 0.02720 -0.18693 -0.47648
H*10 H 0.14537 -0.21217 -0.54997
H*11 H 0.14763 0.39699 -0.46719
C1+ C 0.62861 0.29647 0.21899
N'2+ N 0.59827 0.08153 0.34298
N'3+ N 0.52774 0.06060 0.28668
N'4+ N 0.54443 0.19132 0.20889
N5+ N 0.66154 0.22909 0.30164
C6+ C 0.67849 0.46120 0.15391
N7+ N 0.78840 0.40650 0.08212
O8+ O 0.81459 0.50093 0.00457
O9+ O 0.83762 0.27634 0.11373
N10+ N 0.60202 0.53318 0.08605
O11+ O 0.59245 0.42043 0.01925
O12+ O 0.55954 0.69124 0.10748
N13+ N 0.70087 0.63831 0.21980
O14+ O 0.63778 0.65481 0.30169
O15+ O 0.77642 0.74258 0.18368
O16+ O 0.74656 0.29210 0.33911
```

```
H*17+ H 0.71542 0.36758 0.39986

#END

data_2e_q_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                 12.629
_cell_length_b                 7.750
_cell_length_c                 11.442
_cell_angle_alpha               90.00
_cell_angle_beta                92.37
_cell_angle_gamma                 90.00
_cell_volume                   1118.92
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.73161 0.12020 0.63286
N2 N 0.74582 0.00073 0.54369
H*3 H 0.79352 0.04325 0.48055
N'4 N 0.63756 0.14521 0.67023
N5 N 0.82310 0.20304 0.67330
H*6 H 0.88956 0.13013 0.67081
H*7 H 0.81240 0.26061 0.75188
N8 N 0.63972 0.25865 0.77098
H*9 H 0.62043 0.37936 0.74091
H*10 H 0.57701 0.22172 0.81824
H*11 H 0.67545 -0.04361 0.50987
C1+ C 0.04864 0.22045 0.27500
N'2+ N -0.03553 0.23266 0.43859
N'3+ N -0.04550 0.07937 0.39294
N'4+ N 0.00601 0.06722 0.29153
N5+ N 0.02285 0.32227 0.36539
C6+ C 0.11196 0.27540 0.17546
N7+ N 0.23272 0.29261 0.20814
O8+ O 0.29260 0.27528 0.12914
O9+ O 0.25350 0.32632 0.31036
N10+ N 0.09951 0.14354 0.07377
O11+ O 0.14200 0.00599 0.09314
O12+ O 0.04826 0.19061 -0.01252
N13+ N 0.07447 0.45498 0.12743
```

O14+ O -0.01936 0.48509 0.13758
O15+ O 0.14037 0.54513 0.08391
O16+ O 0.05153 0.48905 0.38513
H*17+ H -0.01169 0.55719 0.36616

#END

data_2e_q_3
_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 9.603
_cell_length_b 7.936
_cell_length_c 15.100
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1150.76
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.12327 0.50440 0.36852
N2 N -0.16085 0.62505 0.43130
H*3 H -0.26255 0.65926 0.42840
N'4 N -0.00853 0.52314 0.32473
N5 N -0.21648 0.37250 0.35910
H*6 H -0.26686 0.34031 0.41558
H*7 H -0.17180 0.27369 0.32686
N8 N 0.02101 0.37746 0.27000
H*9 H -0.01190 0.40591 0.20734
H*10 H 0.12675 0.37262 0.26560
H*11 H -0.09635 0.72623 0.42948
C1+ C 0.48426 0.53629 0.17671
N'2+ N 0.40992 0.53519 0.31399
N'3+ N 0.32480 0.44962 0.26419
N'4+ N 0.36803 0.44739 0.17866
N5+ N 0.50980 0.59057 0.25997
C6+ C 0.57162 0.57419 0.09837
N7+ N 0.71025 0.47158 0.09623
O8+ O 0.76129 0.44756 0.02408
O9+ O 0.75419 0.43007 0.16858
N10+ N 0.49061 0.53425 0.01197

```
O11+ O 0.47258 0.38556 -0.00151
O12+ O 0.45300 0.65430 -0.03174
N13+ N 0.61300 0.76456 0.09568
O14+ O 0.52773 0.85988 0.12820
O15+ O 0.72288 0.79966 0.06114
O16+ O 0.61965 0.68355 0.28876
H*17+ H 0.58310 0.79661 0.29841

#END

data_2e_q_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                 6.194
_cell_length_b                 23.786
_cell_length_c                 7.808
_cell_angle_alpha               90.00
_cell_angle_beta                79.59
_cell_angle_gamma                 90.00
_cell_volume                   1131.42
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.46863 0.92617 0.10037
N2 N 0.44045 0.97638 0.01474
H*3 H 0.34599 0.97252 -0.07809
N'4 N 0.66196 0.91286 0.12785
N5 N 0.27965 0.89457 0.14830
H*6 H 0.14042 0.91758 0.17938
H*7 H 0.29948 0.86513 0.23877
N8 N 0.65560 0.86283 0.23456
H*9 H 0.70011 0.82981 0.15178
H*10 H 0.78201 0.86729 0.30067
H*11 H 0.58643 0.99508 -0.03190
C1+ C 0.03167 0.11298 0.12691
N'2+ N -0.12920 0.03070 0.16648
N'3+ N -0.14649 0.05039 0.01398
N'4+ N -0.04794 0.10131 -0.01495
N5+ N -0.01882 0.06956 0.23862
C6+ C 0.15168 0.16432 0.16214
N7+ N 0.40284 0.15435 0.15139
```

```
O8+ O 0.52076 0.19483 0.11620
O9+ O 0.45259 0.10660 0.18435
N10+ N 0.12369 0.21106 0.02924
O11+ O 0.21930 0.20211 -0.11751
O12+ O 0.00865 0.25070 0.08497
N13+ N 0.06212 0.18775 0.34839
O14+ O -0.13213 0.17893 0.40164
O15+ O 0.19043 0.21271 0.42051
O16+ O 0.03435 0.06333 0.39894
H*17+ H -0.10085 0.07034 0.48147

#END

data_2e_q_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                 10.486
_cell_length_b                 11.411
_cell_length_c                 9.220
_cell_angle_alpha               90.00
_cell_angle_beta                96.43
_cell_angle_gamma               90.00
_cell_volume                   1096.29
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.23787 0.05386 0.27413
N2 N 0.19598 -0.05741 0.22780
H*3 H 0.10884 -0.07931 0.25766
N'4 N 0.35541 0.06781 0.33079
N5 N 0.14563 0.14094 0.25426
H*6 H 0.08068 0.12975 0.16539
H*7 H 0.18660 0.22189 0.26176
N8 N 0.38547 0.19043 0.35740
H*9 H 0.37740 0.20589 0.46526
H*10 H 0.48101 0.19774 0.34821
H*11 H 0.26320 -0.11942 0.25747
C1+ C 0.65158 -0.09873 0.15803
N'2+ N 0.45364 -0.16230 0.11533
N'3+ N 0.50751 -0.16222 -0.00520
N'4+ N 0.63048 -0.12356 0.01747
```

N5+ N 0.54263 -0.12235 0.21810
C6+ C 0.77103 -0.05159 0.23786
N7+ N 0.84779 -0.14475 0.33618
O8+ O 0.96213 -0.12874 0.36191
O9+ O 0.78277 -0.22276 0.37975
N10+ N 0.86092 -0.00404 0.12871
O11+ O 0.90843 -0.07905 0.05916
O12+ O 0.87274 0.10166 0.12335
N13+ N 0.74163 0.05175 0.34023
O14+ O 0.64729 0.10953 0.29703
O15+ O 0.81475 0.06580 0.44994
O16+ O 0.52193 -0.11173 0.36037
H*17+ H 0.46895 -0.04198 0.36495

#END

S39. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

data_2f_q_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 16.442
_cell_length_b 17.904
_cell_length_c 8.136
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 2395.06
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25422 0.66480 -0.22950
N'2 N 0.18087 0.64387 -0.26305
N3 N 0.32037 0.62416 -0.28991
H*4 H 0.36589 0.61878 -0.20665
N5 N 0.27558 0.72550 -0.13255

N6 N 0.30547 0.55515 -0.37005
N7 N 0.12129 0.69567 -0.20016
H*8 H 0.10867 0.68085 -0.08138
H*9 H 0.25364 0.53227 -0.32178
H*10 H 0.29189 0.56717 -0.48931
H*11 H 0.06946 0.68476 -0.26406
H*12 H 0.32879 0.74999 -0.16514
H*13 H 0.22863 0.76229 -0.12283
C1+ C 0.40393 0.11027 0.25139
N'2+ N 0.27568 0.09257 0.31398
N'3+ N 0.28120 0.12760 0.17421
N'4+ N 0.35994 0.13930 0.13152
N5+ N 0.35203 0.08168 0.36377
C6+ C 0.49375 0.10949 0.26499
N7+ N 0.53168 0.03107 0.23115
O8+ O 0.60113 0.03024 0.18212
O9+ O 0.48727 -0.02141 0.26218
N10+ N 0.53168 0.16528 0.14077
O11+ O 0.52608 0.14636 -0.00153
O12+ O 0.56161 0.22150 0.19820
N13+ N 0.52190 0.13314 0.44089
O14+ O 0.47694 0.17713 0.51011
O15+ O 0.58510 0.10697 0.49059
O16+ O 0.37081 0.04532 0.50537
H*17+ H 0.35981 0.08083 0.59336

#END

data_2f_q_2
_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 11.891
_cell_length_b 9.401
_cell_length_c 14.166
_cell_angle_alpha 90.00
_cell_angle_beta 48.53
_cell_angle_gamma 90.00
_cell_volume 1186.58
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

```
C1 C 0.23010 0.64799 0.02432
N'2 N 0.36939 0.67264 -0.07255
N3 N 0.12308 0.64659 0.01165
H*4 H 0.02533 0.69392 0.08488
N5 N 0.17175 0.62420 0.14622
N6 N 0.16683 0.68998 -0.10453
N7 N 0.46378 0.65948 -0.04274
H*8 H 0.46453 0.75571 -0.00936
H*9 H 0.25185 0.76263 -0.14554
H*10 H 0.21354 0.60366 -0.16252
H*11 H 0.56968 0.64689 -0.12709
H*12 H 0.08121 0.55887 0.19754
H*13 H 0.25376 0.59430 0.14654
C1+ C 0.07512 0.12757 0.13253
N'2+ N -0.16223 0.07317 0.24546
N'3+ N -0.14397 0.20996 0.22682
N'4+ N 0.00204 0.24729 0.15680
N5+ N -0.02609 0.02052 0.18734
C6+ C 0.23776 0.11062 0.06055
N7+ N 0.32515 0.04588 -0.07331
O8+ O 0.45722 0.07463 -0.15204
O9+ O 0.25062 -0.03036 -0.08304
N10+ N 0.30965 0.25683 0.04382
O11+ O 0.31794 0.33711 -0.02733
O12+ O 0.34774 0.27568 0.10397
N13+ N 0.26620 0.01015 0.13077
O14+ O 0.16867 0.01265 0.24521
O15+ O 0.38119 -0.05823 0.06652
O16+ O 0.00006 -0.12077 0.18452
H*17+ H -0.03590 -0.14327 0.26773

#END

data_2f_q_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                 14.529
_cell_length_b                 11.260
_cell_length_c                 11.036
_cell_angle_alpha               90.00
_cell_angle_beta               137.60
_cell_angle_gamma                90.00
_cell_volume                   1217.42
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.30487 0.88064 -0.25592
N'2 N -0.37420 0.84409 -0.23096
N3 N -0.28917 1.00231 -0.26171
H*4 H -0.29660 1.02398 -0.35787
N5 N -0.24332 0.80865 -0.28233
N6 N -0.36428 1.08344 -0.26248
N7 N -0.37054 0.71648 -0.21609
H*8 H -0.44770 0.68247 -0.34311
H*9 H -0.45319 1.04322 -0.32260
H*10 H -0.30996 1.09606 -0.13203
H*11 H -0.39813 0.69935 -0.15579
H*12 H -0.15740 0.84361 -0.23556
H*13 H -0.23020 0.72467 -0.23750
C1+ C 0.18976 0.11474 0.71128
N'2+ N 0.10642 0.04951 0.80220
N'3+ N 0.00937 0.09636 0.64299
N'4+ N 0.05750 0.13743 0.58238
N5+ N 0.21983 0.06087 0.84664
C6+ C 0.28985 0.14380 0.71247
N7+ N 0.33683 0.03300 0.68408
O8+ O 0.37630 0.05128 0.62027
O9+ O 0.33173 -0.06052 0.73415
N10+ N 0.22762 0.23429 0.56145
O11+ O 0.13838 0.19410 0.41097
O12+ O 0.27304 0.33455 0.60913
N13+ N 0.42158 0.20083 0.89518
O14+ O 0.40327 0.25846 0.96936
O15+ O 0.52745 0.18431 0.94431
O16+ O 0.34321 0.02003 1.00435
H*17+ H 0.37457 0.07690 1.09529

#END

data_2f_q_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                 9.152
_cell_length_b                 12.108
_cell_length_c                 10.825
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 82.76
_cell_angle_gamma                90.00
_cell_volume                   1189.98
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.28234 0.20949 0.76053
N'2 N 0.35141 0.19317 0.65040
N3 N 0.25432 0.31708 0.80405
H*4 H 0.26876 0.32634 0.89482
N5 N 0.23285 0.12772 0.84552
N6 N 0.31873 0.40654 0.73208
N7 N 0.36031 0.07735 0.61902
H*8 H 0.45186 0.04580 0.65168
H*9 H 0.41574 0.38010 0.68367
H*10 H 0.25143 0.42354 0.66640
H*11 H 0.38307 0.07483 0.52463
H*12 H 0.14065 0.14826 0.90295
H*13 H 0.22479 0.05375 0.80223
C1+ C -0.26120 0.15680 0.81590
N'2+ N -0.29423 0.06327 0.99063
N'3+ N -0.40551 0.04798 0.92861
N'4+ N -0.38838 0.10459 0.81958
N5+ N -0.20349 0.13152 0.92131
C6+ C -0.19268 0.23146 0.71671
N7+ N -0.05921 0.17821 0.63386
O8+ O -0.03164 0.21395 0.52915
O9+ O 0.00563 0.10753 0.68545
N10+ N -0.30742 0.26594 0.62994
O11+ O -0.34336 0.19245 0.56430
O12+ O -0.34971 0.36101 0.63791
N13+ N -0.13416 0.33917 0.77304
O14+ O -0.20347 0.36886 0.87086
O15+ O -0.02866 0.38333 0.71473
O16+ O -0.07273 0.16533 0.95530
H*17+ H -0.09750 0.22087 1.01969

#END

data_2f_q_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 20.231
_cell_length_b 6.144
_cell_length_c 10.588
_cell_angle_alpha 90.00
_cell_angle_beta 109.92
_cell_angle_gamma 90.00
_cell_volume 1237.34
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.61592 0.78065 0.19694
N'2 N 0.64431 0.96164 0.17989
N3 N 0.64797 0.65460 0.31144
H*4 H 0.64598 0.49283 0.29152
N5 N 0.55466 0.69116 0.10827
N6 N 0.71586 0.71476 0.39870
N7 N 0.60107 1.07554 0.06138
H*8 H 0.61344 1.01823 -0.01857
H*9 H 0.74173 0.79086 0.34316
H*10 H 0.70900 0.83083 0.46181
H*11 H 0.61848 1.23206 0.07402
H*12 H 0.52676 0.60197 0.15319
H*13 H 0.52531 0.80615 0.04437
C1+ C 0.32921 0.19088 0.22397
N'2+ N 0.22294 0.06628 0.12003
N'3+ N 0.26357 0.01905 0.05141
N'4+ N 0.32992 0.09349 0.11324
N5+ N 0.26333 0.17447 0.22792
C6+ C 0.38858 0.30239 0.32589
N7+ N 0.41960 0.17011 0.45892
O8+ O 0.48041 0.20529 0.52507
O9+ O 0.37812 0.04843 0.48350
N10+ N 0.44903 0.34370 0.26979
O11+ O 0.47979 0.18112 0.25660
O12+ O 0.45843 0.53121 0.24394
N13+ N 0.36542 0.52781 0.36501
O14+ O 0.31888 0.61797 0.27549
O15+ O 0.39585 0.59257 0.47782
O16+ O 0.23917 0.24821 0.32512
H*17+ H 0.21125 0.37683 0.28743

#END

S40. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 5-(trinitromethyl)tetrazole 1*N*-oxide (cocrystal form).

data_2g_q_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                 10.031
_cell_length_b                 11.978
_cell_length_c                 10.820
_cell_angle_alpha               90.00
_cell_angle_beta                82.55
_cell_angle_gamma                 90.00
_cell_volume                   1289.06
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.22609 0.56425 0.26540
N'2 N -0.30760 0.56283 0.36879
N3 N -0.34482 0.67428 0.41093
N4 N -0.18922 0.66194 0.19971
N5 N -0.07697 0.65567 0.10583
N6 N -0.17276 0.46566 0.21449
N7 N -0.23126 0.36302 0.25682
H*8 H -0.38743 0.66506 0.50085
H*9 H -0.42058 0.70160 0.36349
H*10 H -0.19412 0.72846 0.25902
H*11 H -0.09066 0.71165 0.03812
H*12 H 0.01018 0.67396 0.14070
H*13 H -0.13950 0.46790 0.12225
H*14 H -0.19806 0.34581 0.33991
H*15 H -0.33277 0.37468 0.27830
C1+ C 0.22726 0.89508 -0.19220
N'2+ N 0.14254 0.83076 -0.00903
N'3+ N 0.05228 0.82680 -0.08520
N'4+ N 0.10163 0.86582 -0.19977
N5+ N 0.25225 0.87370 -0.07474
C6+ C 0.32463 0.94432 -0.29195
N7+ N 0.43544 0.86034 -0.34757
O8+ O 0.48657 0.87783 -0.45330
O9+ O 0.46094 0.78708 -0.27638
N10+ N 0.25073 0.98636 -0.40048
O11+ O 0.20752 0.91287 -0.46089
O12+ O 0.24271 1.08684 -0.41229
N13+ N 0.39924 1.04624 -0.24242
O14+ O 0.33372 1.09849 -0.15905
```

O15+ O 0.51241 1.06463 -0.29152
O16+ O 0.36933 0.88904 -0.02637
H*17+ H 0.35521 0.95498 0.02643

#END

data_2g_q_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 14.169
_cell_length_b 9.541
_cell_length_c 9.482
_cell_angle_alpha 90.00
_cell_angle_beta 87.22
_cell_angle_gamma 90.00
_cell_volume 1280.33
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.63938 0.36267 0.71195
N'2 N 0.57235 0.28174 0.67124
N3 N 0.48274 0.31555 0.74212
N4 N 0.62360 0.47492 0.80419
N5 N 0.70376 0.53358 0.86576
N6 N 0.73143 0.34069 0.66222
N7 N 0.74930 0.25451 0.54275
H*8 H 0.44001 0.23280 0.72297
H*9 H 0.45406 0.39904 0.69148
H*10 H 0.56530 0.45662 0.86897
H*11 H 0.69117 0.63709 0.88311
H*12 H 0.71655 0.48618 0.95933
H*13 H 0.77503 0.42418 0.66764
H*14 H 0.74338 0.15325 0.57631
H*15 H 0.69528 0.26767 0.47602
C1+ C -0.08483 0.36334 0.19919
N'2+ N -0.21487 0.48517 0.23624
N'3+ N -0.21925 0.41362 0.11985
N'4+ N -0.13982 0.33658 0.09390
N5+ N -0.13098 0.45501 0.28656
C6+ C 0.01090 0.30674 0.21941
N7+ N 0.01281 0.19353 0.33806

```
O8+ O 0.07638 0.10891 0.32843
O9+ O -0.04936 0.20514 0.43039
N10+ N 0.05143 0.23882 0.08064
O11+ O 0.01316 0.13061 0.04936
O12+ O 0.11541 0.30113 0.01819
N13+ N 0.08045 0.42529 0.26075
O14+ O 0.06342 0.54031 0.21237
O15+ O 0.14442 0.39244 0.33398
O16+ O -0.10146 0.50908 0.40945
H*17+ H -0.08325 0.60549 0.38791

#END

data_2g_q_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                 14.183
_cell_length_b                 12.214
_cell_length_c                 11.143
_cell_angle_alpha               90.00
_cell_angle_beta               136.23
_cell_angle_gamma                90.00
_cell_volume                   1335.32
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.06204 -0.81493 0.65977
N'2 N -0.07178 -0.82319 0.53506
N3 N -0.11541 -0.93124 0.45905
N4 N -0.10021 -0.89840 0.70310
N5 N -0.05521 -0.88960 0.86494
N6 N -0.01359 -0.71954 0.75541
N7 N -0.00681 -0.62319 0.69176
H*8 H -0.09639 -0.93520 0.38694
H*9 H -0.21928 -0.93537 0.37170
H*10 H -0.09062 -0.97277 0.67109
H*11 H -0.12569 -0.92577 0.85385
H*12 H 0.03650 -0.92741 0.96107
H*13 H -0.03998 -0.70711 0.81778
H*14 H 0.07754 -0.62967 0.71633
H*15 H -0.08724 -0.62331 0.55923
```

```
C1+ C 0.36085 0.13279 0.16345
N'2+ N 0.34516 0.06382 0.33016
N'3+ N 0.24504 0.02834 0.17207
N'4+ N 0.25189 0.06931 0.06536
N5+ N 0.41800 0.12955 0.32627
C6+ C 0.41222 0.19809 0.10821
N7+ N 0.54264 0.14840 0.16919
O8+ O 0.56224 0.17083 0.08288
O9+ O 0.61303 0.09405 0.30119
N10+ N 0.30133 0.20697 -0.09254
O11+ O 0.27921 0.12237 -0.16587
O12+ O 0.24815 0.29598 -0.15401
N13+ N 0.44990 0.31692 0.18279
O14+ O 0.38203 0.35264 0.20315
O15+ O 0.53998 0.36240 0.21077
O16+ O 0.53314 0.18100 0.46967
H*17+ H 0.50220 0.24162 0.49111

#END

data_2g_q_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                 13.868
_cell_length_b                 9.863
_cell_length_c                 9.058
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1238.95
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.44909 -0.02121 -0.22458
N'2 N 0.38082 -0.06637 -0.30925
N3 N 0.31419 -0.15134 -0.22892
N4 N 0.45179 -0.04427 -0.07280
N5 N 0.54014 -0.01784 0.00039
N6 N 0.52312 0.05518 -0.28364
N7 N 0.51252 0.11177 -0.42600
H*8 H 0.27508 -0.19992 -0.30774
```

H*9 H 0.26615 -0.09011 -0.17476
H*10 H 0.41698 -0.13241 -0.04761
H*11 H 0.52510 0.01172 0.10529
H*12 H 0.58270 -0.10213 0.00344
H*13 H 0.55906 0.11468 -0.21133
H*14 H 0.52456 0.03575 -0.50001
H*15 H 0.44160 0.13755 -0.44036
C1+ C 0.11349 0.25097 -0.21931
N'2+ N -0.00820 0.13118 -0.13645
N'3+ N -0.03962 0.24334 -0.19499
N'4+ N 0.03398 0.31987 -0.24784
N5+ N 0.08749 0.13502 -0.15049
C6+ C 0.21390 0.29175 -0.25293
N7+ N 0.25864 0.21165 -0.38482
O8+ O 0.32258 0.26764 -0.45219
O9+ O 0.22547 0.09873 -0.40332
N10+ N 0.21807 0.44484 -0.29190
O11+ O 0.18195 0.47355 -0.40940
O12+ O 0.25543 0.51871 -0.20122
N13+ N 0.28146 0.26788 -0.11733
O14+ O 0.24234 0.27935 0.00243
O15+ O 0.36513 0.24253 -0.14294
O16+ O 0.14582 0.03305 -0.10362
H*17+ H 0.14900 0.04232 0.00337

#END

data_2g_q_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 9.115
_cell_length_b 14.136
_cell_length_c 9.687
_cell_angle_alpha 90.00
_cell_angle_beta 93.27
_cell_angle_gamma 90.00
_cell_volume 1246.13
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.76711 0.72131 0.19009

N'2 N 0.73833 0.73816 0.31738
N3 N 0.67672 0.65626 0.38182
N4 N 0.75080 0.63237 0.12901
N5 N 0.75219 0.62820 -0.01709
N6 N 0.81834 0.79300 0.10874
N7 N 0.87328 0.87687 0.17190
H*8 H 0.63453 0.68102 0.46977
H*9 H 0.76111 0.61222 0.41407
H*10 H 0.67155 0.59466 0.17499
H*11 H 0.79471 0.56474 -0.04343
H*12 H 0.64878 0.63460 -0.06216
H*13 H 0.87276 0.77186 0.02607
H*14 H 0.78468 0.91642 0.19573
H*15 H 0.92427 0.85951 0.26544
C1+ C 0.24237 0.09089 0.28681
N'2+ N 0.03976 0.08078 0.39751
N'3+ N 0.00871 0.07810 0.26471
N'4+ N 0.13196 0.08396 0.19298
N5+ N 0.18552 0.08914 0.41262
C6+ C 0.40048 0.10056 0.26187
N7+ N 0.49004 0.00821 0.29351
O8+ O 0.60090 -0.00207 0.23220
O9+ O 0.43975 -0.04287 0.38017
N10+ N 0.42032 0.12735 0.10871
O11+ O 0.39059 0.06454 0.02700
O12+ O 0.46118 0.20746 0.08711
N13+ N 0.47378 0.18003 0.35430
O14+ O 0.39232 0.24489 0.38148
O15+ O 0.60275 0.17081 0.38826
O16+ O 0.25943 0.09268 0.53836
H*17+ H 0.24354 0.15632 0.57315

#END

S41. Optimized crystal structure coordinates for 5 polymorphs of Ammonia - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

data_3a_q_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 16.336
_cell_length_b 8.454
_cell_length_c 6.810
_cell_angle_alpha 90.00

```
_cell_angle_beta                66.20
_cell_angle_gamma               90.00
_cell_volume                    860.512
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.25923 0.97954 0.28964
H*2 H -0.20345 0.91036 0.24115
H*3 H -0.24015 1.08572 0.21405
H*4 H -0.30150 0.92890 0.23140
C1+ C 0.15688 -0.02588 0.22309
N'2+ N 0.12059 -0.14990 0.16691
C3+ C 0.24375 -0.02094 0.23944
C4+ C 0.39965 -0.01436 0.26232
N'5+ N 0.04162 -0.10127 0.17116
N'6+ N 0.02706 0.04773 0.22721
N7+ N 0.09850 0.09492 0.25892
N'8+ N 0.28146 0.12166 0.22141
N9+ N 0.36079 0.12283 0.23507
N10+ N 0.35536 -0.15511 0.27824
N'11+ N 0.27545 -0.16092 0.26844
O12+ O 0.10534 0.24528 0.32376
O13+ O 0.39229 -0.27892 0.30399
O14+ O 0.40219 0.25042 0.22191
N15+ N 0.47925 -0.01133 0.27432
H*16+ H 0.50581 -0.11524 0.29340
H*17+ H 0.50988 0.09448 0.26110
H*18+ H 0.04709 0.29162 0.35175

#END

data_3a_q_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                  19.751
_cell_length_b                  8.500
_cell_length_c                  6.661
_cell_angle_alpha               90.00
_cell_angle_beta                50.42
_cell_angle_gamma               90.00
_cell_volume                    861.892
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.49289 -0.22459 0.80553
H*2 H 0.50120 -0.33461 0.73206
H*3 H 0.55388 -0.17642 0.70447
H*4 H 0.46043 -0.16037 0.76107
C1+ C -0.09324 0.22412 0.81097
N'2+ N -0.13172 0.09953 0.79934
C3+ C -0.00558 0.22952 0.73705
C4+ C 0.15154 0.23682 0.59819
N'5+ N -0.21065 0.14784 0.88275
N'6+ N -0.22309 0.29718 0.94558
N7+ N -0.15034 0.34491 0.90063
N'8+ N 0.03259 0.37097 0.67410
N9+ N 0.11259 0.37256 0.60550
N10+ N 0.10672 0.09717 0.66579
N'11+ N 0.02620 0.09105 0.73896
O12+ O -0.14108 0.49582 0.94990
O13+ O 0.14377 -0.02530 0.65839
O14+ O 0.15451 0.49919 0.54417
N15+ N 0.23178 0.24023 0.52761
H*16+ H 0.25837 0.13738 0.52351
H*17+ H 0.26277 0.34519 0.47832
H*18+ H -0.19863 0.54242 1.03515

#END

data_3a_q_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                 18.823
_cell_length_b                 8.613
_cell_length_c                 6.460
_cell_angle_alpha               90.00
_cell_angle_beta                56.98
_cell_angle_gamma                 90.00
_cell_volume                   878.15
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.06340 0.72383 0.35512
H*2 H -0.00434 0.67609 0.26522
H*3 H -0.05842 0.82618 0.26901
H*4 H -0.10016 0.65231 0.32560
C1+ C 0.40476 0.20821 0.31549
N'2+ N 0.36210 0.08502 0.31385
C3+ C 0.49407 0.21268 0.23704
C4+ C 0.65375 0.21823 0.09065
N'5+ N 0.28304 0.13371 0.39803
N'6+ N 0.27450 0.28195 0.45181
N7+ N 0.34990 0.32856 0.40020
N'8+ N 0.53193 0.35139 0.16929
N9+ N 0.61334 0.35215 0.09678
N10+ N 0.60907 0.08134 0.16339
N'11+ N 0.52736 0.07618 0.24035
O12+ O 0.36377 0.47820 0.43891
O13+ O 0.64752 -0.03950 0.15692
O14+ O 0.65523 0.47628 0.03065
N15+ N 0.73532 0.22076 0.01622
H*16+ H 0.76289 0.11930 0.01325
H*17+ H 0.76611 0.32366 -0.03673
H*18+ H 0.30770 0.52528 0.52240

#END

data_3a_q_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                  10.211
_cell_length_b                  8.492
_cell_length_c                  14.124
_cell_angle_alpha                 90.00
_cell_angle_beta                 45.77
_cell_angle_gamma                    90.00
_cell_volume                    877.566
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

N1 N -0.01876 0.25520 0.65861
H*2 H 0.10655 0.30597 0.60316
H*3 H -0.08959 0.32245 0.64716
H*4 H 0.00172 0.14846 0.61707
C1+ C -0.18311 0.74163 0.15123
N'2+ N -0.25360 0.61941 0.13999
C3+ C -0.00778 0.74623 0.11329
C4+ C 0.30700 0.75235 0.04199
N'5+ N -0.41414 0.66767 0.18510
N'6+ N -0.44684 0.81474 0.22383
N7+ N -0.30367 0.86105 0.20261
N'8+ N 0.06678 0.88853 0.08770
N9+ N 0.22695 0.88943 0.05236
N10+ N 0.21914 0.61195 0.07007
N'11+ N 0.05777 0.60634 0.10752
O12+ O -0.29330 1.00928 0.23435
O13+ O 0.29511 0.48821 0.06029
O14+ O 0.30911 1.01668 0.02686
N15+ N 0.46773 0.75515 0.00573
H*16+ H 0.52258 0.65135 -0.00138
H*17+ H 0.52842 0.86072 -0.01459
H*18+ H -0.41236 1.05477 0.28009

#END

data_3a_q_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 9.522
_cell_length_b 8.590
_cell_length_c 15.860
_cell_angle_alpha 90.00
_cell_angle_beta 136.81
_cell_angle_gamma 90.00
_cell_volume 887.865
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.24817 0.80196 -0.31164
H*2 H 0.18373 0.69507 -0.34858
H*3 H 0.26572 0.85034 -0.36218

H*4 H 0.14301 0.86799 -0.32632
C1+ C 0.11794 0.23268 0.65191
N'2+ N 0.02987 0.10798 0.64807
C3+ C 0.21579 0.24142 0.61148
C4+ C 0.38469 0.25472 0.53609
N'5+ N -0.04099 0.15271 0.69280
N'6+ N -0.00131 0.29993 0.72422
N7+ N 0.09668 0.34995 0.69866
N'8+ N 0.22706 0.38284 0.58155
N9+ N 0.31518 0.38751 0.54410
N10+ N 0.36502 0.11481 0.56868
N'11+ N 0.28054 0.10564 0.60821
O12+ O 0.16543 0.49956 0.72224
O13+ O 0.43069 -0.00493 0.56096
O14+ O 0.33551 0.51442 0.51443
N15+ N 0.47128 0.26119 0.49774
H*16+ H 0.51962 0.16046 0.49257
H*17+ H 0.48228 0.36623 0.47415
H*18+ H 0.13874 0.54340 0.76612

#END

S42. Optimized crystal structure coordinates for 5 polymorphs of Hydroxylamine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

data_3b_q_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 19.526
_cell_length_b 6.258
_cell_length_c 7.540
_cell_angle_alpha 90.00
_cell_angle_beta 96.11
_cell_angle_gamma 90.00
_cell_volume 916.107
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.01451 -0.70374 -0.62524
H*2 H -0.01345 -0.71824 -0.75995
H*3 H -0.04522 -0.57471 -0.60809

O4 O 0.05392 -0.63004 -0.56200
H*5 H 0.06922 -0.73527 -0.47292
C1+ C 0.62784 0.23446 -0.12147
N'2+ N 0.57095 0.27543 -0.23039
C3+ C 0.69809 0.21211 -0.17175
C4+ C 0.82290 0.17818 -0.26432
N'5+ N 0.51876 0.28434 -0.12806
N'6+ N 0.54059 0.25106 0.04000
N7+ N 0.60820 0.22068 0.04460
N'8+ N 0.74924 0.24813 -0.04278
N9+ N 0.81264 0.22852 -0.09225
N10+ N 0.76670 0.14506 -0.38707
N'11+ N 0.70256 0.16016 -0.34225
O12+ O 0.64800 0.17713 0.20035
O13+ O 0.77754 0.09832 -0.54355
O14+ O 0.86473 0.25717 0.01821
N15+ N 0.88661 0.16048 -0.31194
H*16+ H 0.89195 0.12413 -0.44041
H*17+ H 0.92663 0.18683 -0.21794
H*18+ H 0.61466 0.16033 0.28669

#END

data_3b_q_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 9.831
_cell_length_b 6.401
_cell_length_c 14.639
_cell_angle_alpha 90.00
_cell_angle_beta 98.14
_cell_angle_gamma 90.00
_cell_volume 911.925
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.55082 0.14455 0.08479
H*2 H 0.59309 0.01132 0.06251
H*3 H 0.54533 0.12099 0.15324
O4 O 0.40918 0.13623 0.04178
H*5 H 0.39793 0.26766 0.00928

C1+ C -0.26549 -0.13849 0.66967
N'2+ N -0.38137 -0.12017 0.61062
C3+ C -0.12543 -0.15523 0.64642
C4+ C 0.12310 -0.17976 0.60320
N'5+ N -0.48443 -0.10762 0.66160
N'6+ N -0.43796 -0.11698 0.74989
N7+ N -0.30226 -0.13552 0.75513
N'8+ N -0.02389 -0.09734 0.71212
N9+ N 0.10245 -0.11239 0.68901
N10+ N 0.01145 -0.23490 0.54045
N'11+ N -0.11620 -0.22488 0.56136
O12+ O -0.21978 -0.15351 0.83797
O13+ O 0.03330 -0.29687 0.46248
O14+ O 0.20598 -0.06366 0.74556
N15+ N 0.25000 -0.19269 0.58096
H*16+ H 0.26075 -0.24215 0.51677
H*17+ H 0.32946 -0.14997 0.62889
H*18+ H -0.28449 -0.16489 0.88234

#END

data_3b_q_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 6.776
_cell_length_b 8.572
_cell_length_c 15.757
_cell_angle_alpha 90.00
_cell_angle_beta 80.99
_cell_angle_gamma 90.00
_cell_volume 903.935
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.05166 -0.06380 0.25237
H*2 H -0.10281 -0.17225 0.27178
H*3 H 0.08418 -0.08141 0.21514
O4 O -0.00257 0.00678 0.32973
H*5 H -0.07963 0.10192 0.33398
C1+ C -0.09076 0.42902 0.34343
N'2+ N -0.14846 0.29869 0.38658

C3+ C 0.00727 0.44047 0.25370
C4+ C 0.17735 0.45775 0.09321
N'5+ N -0.23264 0.34257 0.46586
N'6+ N -0.23031 0.49458 0.47406
N7+ N -0.14298 0.54853 0.39822
N'8+ N -0.01243 0.57641 0.21432
N9+ N 0.07669 0.58343 0.13254
N10+ N 0.18817 0.32295 0.13942
N'11+ N 0.10355 0.31207 0.22159
O12+ O -0.11180 0.70429 0.38397
O13+ O 0.28194 0.20980 0.10194
O14+ O 0.06935 0.70591 0.08928
N15+ N 0.26460 0.46632 0.01124
H*16+ H 0.33654 0.37073 -0.01551
H*17+ H 0.25267 0.56732 -0.02070
H*18+ H -0.15194 0.75086 0.44042

#END

data_3b_q_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 6.161
_cell_length_b 12.628
_cell_length_c 11.877
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 924.044
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.40896 0.50880 -0.08334
H*2 H 0.51900 0.45957 -0.04582
H*3 H 0.31467 0.46118 -0.13285
O4 O 0.53720 0.56848 -0.16311
H*5 H 0.50662 0.64082 -0.14227
C1+ C 0.59162 -0.05324 -0.11250
N'2+ N 0.61449 -0.13820 -0.17822
C3+ C 0.69053 0.05132 -0.12948
C4+ C 0.86451 0.23743 -0.16317

N'5+ N 0.49460 -0.21560 -0.13188
N'6+ N 0.39761 -0.18266 -0.04020
N7+ N 0.45692 -0.08197 -0.02813
N'8+ N 0.58990 0.13306 -0.08060
N9+ N 0.68204 0.22742 -0.09807
N10+ N 0.95496 0.14829 -0.21003
N'11+ N 0.86954 0.05246 -0.19323
O12+ O 0.38822 -0.02259 0.06103
O13+ O 1.12254 0.15964 -0.26892
O14+ O 0.60241 0.30987 -0.05552
N15+ N 0.95391 0.33242 -0.18042
H*16+ H 1.08783 0.33645 -0.22944
H*17+ H 0.88210 0.39617 -0.14486
H*18+ H 0.31179 -0.07332 0.10841

#END

data_3b_q_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 9.840
_cell_length_b 7.494
_cell_length_c 6.456
_cell_angle_alpha 100.48
_cell_angle_beta 83.13
_cell_angle_gamma 97.18
_cell_volume 462.163
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.02731 -0.16252 0.31085
H*2 H -0.08875 -0.12115 0.44596
H*3 H -0.02489 -0.29955 0.30328
O4 O 0.10935 -0.08452 0.36022
H*5 H 0.13976 -0.01566 0.24749
C1+ C 0.25784 0.33642 0.22981
N'2+ N 0.14565 0.22213 0.18668
C3+ C 0.39782 0.28755 0.22921
C4+ C 0.64666 0.19713 0.22202
N'5+ N 0.04121 0.32513 0.20387
N'6+ N 0.08330 0.49874 0.25552
N7+ N 0.21759 0.50623 0.27114
N'8+ N 0.50044 0.41831 0.20084

N9+ N 0.62681 0.37000 0.19917
N10+ N 0.53400 0.07248 0.24955
N'11+ N 0.40607 0.11625 0.25514
O12+ O 0.29536 0.66814 0.32718
O13+ O 0.55507 -0.08467 0.27094
O14+ O 0.73120 0.48226 0.17520
N15+ N 0.77370 0.15062 0.21868
H*16+ H 0.78392 0.02143 0.23503
H*17+ H 0.85397 0.24596 0.19729
H*18+ H 0.22797 0.75649 0.36322

#END

S43. Optimized crystal structure coordinates for 5 polymorphs of Hydrazine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

data_3c_q_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 15.926
_cell_length_b 8.822
_cell_length_c 6.787
_cell_angle_alpha 90.00
_cell_angle_beta 75.90
_cell_angle_gamma 90.00
_cell_volume 924.839
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.21818 0.06911 -0.26047
H*2 H -0.21788 0.09685 -0.11473
H*3 H -0.19469 0.15934 -0.35024
N4 N -0.30408 0.03914 -0.28263
H*5 H -0.31606 -0.07311 -0.25563
H*6 H -0.34985 0.09844 -0.18032
C1+ C 0.65993 -0.09871 0.26432
N'2+ N 0.61869 -0.23094 0.27093
C3+ C 0.75073 -0.07580 0.26911
C4+ C 0.91314 -0.03844 0.27296
N'5+ N 0.53740 -0.19897 0.26076
N'6+ N 0.52611 -0.05258 0.24778

N7+ N 0.60200 0.00985 0.24938
N'8+ N 0.78723 0.05389 0.18931
N9+ N 0.87005 0.07146 0.19397
N10+ N 0.86967 -0.16808 0.35068
N'11+ N 0.78659 -0.18891 0.35143
O12+ O 0.61346 0.16325 0.24170
O13+ O 0.91057 -0.26666 0.42283
O14+ O 0.91085 0.18953 0.12453
N15+ N 0.99609 -0.01957 0.27536
H*16+ H 1.02564 -0.10370 0.33406
H*17+ H 1.02592 0.07712 0.21606
H*18+ H 0.55547 0.20280 0.25156

#END

data_3c_q_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 16.720
_cell_length_b 9.061
_cell_length_c 6.321
_cell_angle_alpha 90.00
_cell_angle_beta 70.52
_cell_angle_gamma 90.00
_cell_volume 902.814
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.45563 0.64833 0.25667
H*2 H -0.45224 0.59211 0.11413
H*3 H -0.44445 0.57532 0.36571
N4 N -0.53824 0.71087 0.36389
H*5 H -0.53849 0.81334 0.29858
H*6 H -0.58486 0.65069 0.33365
C1+ C 0.40155 0.16354 0.31603
N'2+ N 0.35253 0.04464 0.33579
C3+ C 0.49465 0.16787 0.23073
C4+ C 0.66039 0.17297 0.07315
N'5+ N 0.27182 0.09150 0.41844
N'6+ N 0.26830 0.23447 0.45084
N7+ N 0.34860 0.27951 0.38694

N'8+ N 0.52991 0.29746 0.14981
N9+ N 0.61467 0.29821 0.07154
N10+ N 0.61790 0.04505 0.15948
N'11+ N 0.53333 0.04035 0.24216
O12+ O 0.36898 0.42409 0.40192
O13+ O 0.66133 -0.06791 0.15975
O14+ O 0.65474 0.41426 -0.00715
N15+ N 0.74509 0.17530 -0.00701
H*16+ H 0.77644 0.08036 -0.00377
H*17+ H 0.77402 0.27141 -0.06989
H*18+ H 0.31455 0.47052 0.47989

#END

data_3c_q_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 31.112
_cell_length_b 8.856
_cell_length_c 6.811
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1876.62
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.64263 0.93071 0.10452
H*2 H 0.64207 0.90095 -0.04013
H*3 H 0.65625 0.84430 0.18064
N4 N 0.60018 0.95359 0.18194
H*5 H 0.59236 1.06382 0.16031
H*6 H 0.57781 0.88921 0.11131
C1+ C 0.07941 0.39268 0.35025
N'2+ N 0.05874 0.26128 0.33386
C3+ C 0.12467 0.41469 0.40413
C4+ C 0.20562 0.45048 0.49581

N'5+ N 0.01826 0.29388 0.28004
N'6+ N 0.01276 0.43984 0.26181
N7+ N 0.05063 0.50137 0.30469
N'8+ N 0.14277 0.54382 0.34504
N9+ N 0.18405 0.56060 0.39447
N10+ N 0.18405 0.32147 0.54908
N'11+ N 0.14264 0.30143 0.50488
O12+ O 0.05649 0.65411 0.30407
O13+ O 0.20451 0.22267 0.64248
O14+ O 0.20431 0.67808 0.34794
N15+ N 0.24697 0.46855 0.54306
H*16+ H 0.26176 0.38430 0.61703
H*17+ H 0.26176 0.56481 0.50061
H*18+ H 0.02768 0.69397 0.28282

#END

data_3c_q_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 31.826
_cell_length_b 8.671
_cell_length_c 6.840
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1887.59
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.59632 0.44344 -0.22228
H*2 H 0.57803 0.36790 -0.29866
H*3 H 0.59089 0.55085 -0.27629
N4 N 0.64032 0.41144 -0.24564
H*5 H 0.64876 0.33583 -0.13902
H*6 H 0.64673 0.36128 -0.37721
C1+ C 0.08107 0.88606 -0.19541

N'2+ N 0.06211 0.75392 -0.14855
C3+ C 0.12637 0.91788 -0.18960
C4+ C 0.20724 0.97026 -0.18238
N'5+ N 0.02078 0.77570 -0.17706
N'6+ N 0.01311 0.91558 -0.23996
N7+ N 0.05043 0.98414 -0.25201
N'8+ N 0.14003 1.03191 -0.30472
N9+ N 0.18139 1.05774 -0.29801
N10+ N 0.19001 0.85520 -0.06991
N'11+ N 0.14877 0.82728 -0.07047
O12+ O 0.05426 1.13409 -0.31003
O13+ O 0.21437 0.77721 0.03525
O14+ O 0.19773 1.16291 -0.39906
N15+ N 0.24856 0.99689 -0.17822
H*16+ H 0.26656 0.92925 -0.09169
H*17+ H 0.26006 1.08220 -0.26360
H*18+ H 0.02530 1.16959 -0.31999

#END

data_3c_q_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 16.669
_cell_length_b 9.091
_cell_length_c 6.311
_cell_angle_alpha 90.00
_cell_angle_beta 109.31
_cell_angle_gamma 90.00
_cell_volume 902.554
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.46044 -0.34579 0.68934
H*2 H 0.45914 -0.39726 0.83180
H*3 H 0.45045 -0.42325 0.56711
N4 N 0.54141 -0.27867 0.71837
H*5 H 0.53944 -0.17452 0.77514
H*6 H 0.58992 -0.33268 0.83455
C1+ C -0.09730 0.66626 0.12114
N'2+ N -0.14531 0.54803 0.04225

C3+ C -0.00435 0.67027 0.22268
C4+ C 0.16134 0.67484 0.39791
N'5+ N -0.22620 0.59495 -0.03686
N'6+ N -0.23080 0.73732 -0.01113
N7+ N -0.15099 0.78191 0.08618
N'8+ N 0.03292 0.79954 0.21579
N9+ N 0.11755 0.80001 0.30759
N10+ N 0.11690 0.54726 0.39576
N'11+ N 0.03226 0.54283 0.30852
O12+ O -0.13190 0.92578 0.14230
O13+ O 0.15855 0.43434 0.48039
O14+ O 0.15935 0.91575 0.31218
N15+ N 0.24600 0.67690 0.48780
H*16+ H 0.27593 0.58202 0.55167
H*17+ H 0.27643 0.77276 0.48542
H*18+ H -0.18734 0.97209 0.11047

#END

S44. Optimized crystal structure coordinates for 5 polymorphs of Guanidine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

data_3d_q_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 14.898
_cell_length_b 7.615
_cell_length_c 5.722
_cell_angle_alpha 64.58
_cell_angle_beta 116.43
_cell_angle_gamma 92.10
_cell_volume 515.365
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.20282 -0.29932 0.26061
N'2 N 0.11123 -0.33204 0.18015
H*3 H 0.09931 -0.42889 0.09422
N4 N 0.23131 -0.15461 0.35341
H*5 H 0.30196 -0.19169 0.52763
H*6 H 0.17665 -0.10117 0.37832
N7 N 0.28354 -0.39619 0.27105
H*8 H 0.26263 -0.48284 0.16947

H*9 H 0.33197 -0.30974 0.21973
C1+ C 0.58734 -0.24635 0.08537
N'2+ N 0.51630 -0.27158 -0.13777
C3+ C 0.69422 -0.23616 0.15425
C4+ C 0.88351 -0.21382 0.26775
N'5+ N 0.42976 -0.26980 -0.11847
N'6+ N 0.44360 -0.24426 0.10667
N7+ N 0.54111 -0.22912 0.23298
N'8+ N 0.74113 -0.14185 0.31293
N9+ N 0.83804 -0.13318 0.37057
N10+ N 0.82834 -0.30710 0.10536
N'11+ N 0.73184 -0.32131 0.04667
O12+ O 0.58302 -0.20483 0.48076
O13+ O 0.87196 -0.38036 0.01486
O14+ O 0.88997 -0.04934 0.51991
N15+ N 0.98026 -0.20283 0.32573
H*16+ H 1.01081 -0.26335 0.24457
H*17+ H 1.01820 -0.13235 0.44500
H*18+ H 0.52897 -0.21824 0.53561

#END

data_3d_q_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 8.802
_cell_length_b 11.209
_cell_length_c 13.809
_cell_angle_alpha 90.00
_cell_angle_beta 131.22
_cell_angle_gamma 90.00
_cell_volume 1024.79
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.70248 0.35159 -0.08917
N'2 N 0.61820 0.36530 -0.04151
H*3 H 0.58104 0.45241 -0.04513
N4 N 0.78501 0.24170 -0.08039
H*5 H 0.76130 0.21718 -0.16009
H*6 H 0.74949 0.17674 -0.04721

N7 N 0.72287 0.43696 -0.15386
H*8 H 0.68937 0.52123 -0.14721
H*9 H 0.85252 0.43179 -0.13823
C1+ C 0.11785 0.33906 0.71560
N'2+ N 0.03018 0.24859 0.72542
C3+ C 0.21221 0.33515 0.65907
C4+ C 0.37494 0.32638 0.55510
N'5+ N -0.03702 0.29224 0.78184
N'6+ N 0.00456 0.40604 0.80751
N7+ N 0.10004 0.43541 0.76624
N'8+ N 0.22453 0.43892 0.61690
N9+ N 0.30945 0.43283 0.56494
N10+ N 0.35454 0.22458 0.60108
N'11+ N 0.27315 0.22726 0.65530
O12+ O 0.16976 0.54839 0.77994
O13+ O 0.41650 0.12835 0.59133
O14+ O 0.33037 0.52502 0.52287
N15+ N 0.45837 0.32165 0.50217
H*16+ H 0.50381 0.24127 0.49616
H*17+ H 0.47004 0.39841 0.46902
H*18+ H 0.14551 0.58866 0.83117

#END

data_3d_q_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 7.440
_cell_length_b 19.239
_cell_length_c 7.559
_cell_angle_alpha 90.00
_cell_angle_beta 97.91
_cell_angle_gamma 90.00
_cell_volume 1071.69
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.54260 -0.35246 0.03964
N'2 N 0.60020 -0.28953 0.03882
H*3 H 0.72862 -0.28524 0.10550
N4 N 0.36302 -0.36806 -0.02697

H*5 H 0.34539 -0.41262 -0.09880
H*6 H 0.29758 -0.32688 -0.08978
N7 N 0.64196 -0.41152 0.10077
H*8 H 0.76478 -0.40125 0.17114
H*9 H 0.57153 -0.44797 0.15955
C1+ C 0.13001 0.63213 0.29002
N'2+ N -0.02359 0.66555 0.23052
C3+ C 0.15811 0.55659 0.29593
C4+ C 0.20556 0.42194 0.30099
N'5+ N 0.01252 0.73380 0.24806
N'6+ N 0.18199 0.74447 0.31564
N7+ N 0.25531 0.68156 0.34133
N'8+ N 0.32894 0.53477 0.29783
N9+ N 0.35071 0.46583 0.30172
N10+ N 0.03510 0.44972 0.29825
N'11+ N 0.00811 0.51832 0.29688
O12+ O 0.43213 0.67287 0.41425
O13+ O -0.09538 0.40837 0.29835
O14+ O 0.50563 0.43938 0.30512
N15+ N 0.22944 0.35312 0.30379
H*16+ H 0.11869 0.32254 0.30223
H*17+ H 0.35686 0.33467 0.30507
H*18+ H 0.47214 0.71976 0.44877

#END

data_3d_q_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 5.334
_cell_length_b 18.074
_cell_length_c 11.263
_cell_angle_alpha 90.00
_cell_angle_beta 103.79
_cell_angle_gamma 90.00
_cell_volume 1054.53
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.28910 0.08367 0.27227
N'2 N 0.18599 0.05084 0.34999

H*3 H 0.03219 0.07992 0.36468
N4 N 0.51897 0.05734 0.24967
H*5 H 0.52799 0.05876 0.16081
H*6 H 0.57004 0.00765 0.28980
N7 N 0.19556 0.14593 0.20174
H*8 H 0.04923 0.17225 0.22707
H*9 H 0.33282 0.18109 0.18672
C1+ C 0.50858 0.30554 0.07696
N'2+ N 0.31880 0.29453 0.13364
C3+ C 0.63244 0.24944 0.01582
C4+ C 0.84541 0.14876 -0.09492
N'5+ N 0.26346 0.36080 0.17497
N'6+ N 0.41009 0.41272 0.14643
N7+ N 0.56173 0.37868 0.08538
N'8+ N 0.74616 0.27412 -0.07023
N9+ N 0.85556 0.22195 -0.12519
N10+ N 0.72269 0.12916 -0.00531
N'11+ N 0.61428 0.17975 0.05292
O12+ O 0.74471 0.41629 0.04311
O13+ O 0.71708 0.06178 0.02097
O14+ O 0.96982 0.23877 -0.20697
N15+ N 0.95434 0.09721 -0.15124
H*16+ H 0.94142 0.04380 -0.12665
H*17+ H 1.04199 0.11381 -0.21700
H*18+ H 0.74065 0.46578 0.07687

#END

data_3d_q_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 11.234
_cell_length_b 6.712
_cell_length_c 14.350
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1082.03
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

C1 C 0.20615 -0.21782 -0.15950
N'2 N 0.25567 -0.21731 -0.24020
H*3 H 0.19655 -0.17884 -0.29109
N4 N 0.26805 -0.28773 -0.08191
H*5 H 0.25562 -0.20792 -0.02274
H*6 H 0.35504 -0.31319 -0.09623
N7 N 0.09151 -0.15214 -0.13702
H*8 H 0.03875 -0.12542 -0.19276
H*9 H 0.04986 -0.23120 -0.08642
C1+ C -0.32361 -0.25067 0.78282
N'2+ N -0.29312 -0.27414 0.87200
C3+ C -0.24257 -0.23083 0.70309
C4+ C -0.09632 -0.20062 0.56212
N'5+ N -0.39497 -0.28775 0.92060
N'6+ N -0.48772 -0.27412 0.86566
N7+ N -0.44379 -0.25168 0.78019
N'8+ N -0.28703 -0.28024 0.61984
N9+ N -0.21126 -0.26247 0.54855
N10+ N -0.05930 -0.15407 0.65073
N'11+ N -0.13279 -0.16717 0.72355
O12+ O -0.51634 -0.22880 0.70465
O13+ O 0.04628 -0.09706 0.66116
O14+ O -0.24355 -0.30341 0.46690
N15+ N -0.02144 -0.18482 0.49020
H*16+ H 0.06278 -0.13961 0.50325
H*17+ H -0.05189 -0.22115 0.42612
H*18+ H -0.59561 -0.21854 0.73175

#END

S45. Optimized crystal structure coordinates for 5 polymorphs of Aminoguanidine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

data_3e_q_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 9.970
_cell_length_b 11.313
_cell_length_c 9.070
_cell_angle_alpha 48.57
_cell_angle_beta 44.75
_cell_angle_gamma 59.33
_cell_volume 538.426
loop_
_atom_site_label
_atom_site_type_symbol

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.28745 -0.40439 -0.05557
N2 N 0.33705 -0.31399 -0.04833
H*3 H 0.36383 -0.20157 -0.18845
N'4 N 0.36319 -0.54750 -0.01022
N5 N 0.15787 -0.32841 -0.11346
H*6 H 0.06188 -0.24959 -0.05498
H*7 H 0.09853 -0.40734 -0.06920
N8 N 0.27965 -0.62869 0.00022
H*9 H 0.37021 -0.62199 -0.16374
H*10 H 0.28992 -0.74502 0.11716
H*11 H 0.44524 -0.36950 -0.02811
C1+ C -0.38911 0.11062 0.67387
N'2+ N -0.38215 -0.02597 0.70771
C3+ C -0.26062 0.15355 0.65686
C4+ C -0.02700 0.22832 0.62149
N'5+ N -0.52456 -0.01333 0.70924
N'6+ N -0.61996 0.12525 0.67747
N7+ N -0.53603 0.20252 0.65481
N'8+ N -0.24662 0.30816 0.53975
N9+ N -0.12765 0.34410 0.52502
N10+ N -0.05124 0.07261 0.73769
N'11+ N -0.17079 0.03194 0.75916
O12+ O -0.60147 0.35184 0.62337
O13+ O 0.04210 -0.03106 0.82523
O14+ O -0.10415 0.48581 0.42048
N15+ N 0.09229 0.26618 0.60394
H*16+ H 0.16457 0.17721 0.67649
H*17+ H 0.10678 0.38206 0.51629
H*18+ H -0.71878 0.37153 0.64206

#END

data_3e_q_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                 12.767
_cell_length_b                 17.603
_cell_length_c                 5.032
_cell_angle_alpha               90.00
_cell_angle_beta               102.11
_cell_angle_gamma                90.00
```

```
_cell_volume                    1105.71
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.34489 0.58182 0.99062
N2 N 0.24109 0.55935 1.00132
H*3 H 0.22866 0.55379 1.19301
N'4 N 0.39400 0.54807 0.82365
N5 N 0.38615 0.63993 1.16716
H*6 H 0.33086 0.67781 1.20226
H*7 H 0.45121 0.66397 1.11355
N8 N 0.49555 0.58423 0.81880
H*9 H 0.55361 0.55319 0.94336
H*10 H 0.50797 0.57498 0.62806
H*11 H 0.21882 0.51215 0.88786
C1+ C 0.28470 0.29915 0.64035
N'2+ N 0.20279 0.28301 0.75743
C3+ C 0.35001 0.24472 0.52467
C4+ C 0.46337 0.14672 0.31438
N'5+ N 0.16603 0.34960 0.83094
N'6+ N 0.22129 0.40662 0.76452
N7+ N 0.29471 0.37555 0.64567
N'8+ N 0.39997 0.27191 0.33643
N9+ N 0.45813 0.22114 0.23274
N10+ N 0.40857 0.12449 0.50885
N'11+ N 0.35083 0.17374 0.62011
O12+ O 0.36848 0.41886 0.55408
O13+ O 0.41507 0.05607 0.58073
O14+ O 0.50926 0.24040 0.05558
N15+ N 0.52134 0.09655 0.20751
H*16+ H 0.52267 0.04211 0.27230
H*17+ H 0.56019 0.11504 0.06420
H*18+ H 0.35645 0.46980 0.61718

#END

data_3e_q_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                  13.838
_cell_length_b                  8.157
_cell_length_c                  6.882
_cell_angle_alpha                 135.29
```

```
_cell_angle_beta                87.11
_cell_angle_gamma               99.01
_cell_volume                   537.686
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24975 0.19616 0.02887
N2 N 0.30097 0.01530 -0.07945
H*3 H 0.27075 -0.08679 -0.05023
N'4 N 0.29810 0.40613 0.16779
N5 N 0.14867 0.12962 -0.02497
H*6 H 0.12557 -0.03927 -0.20887
H*7 H 0.11729 0.25174 0.00811
N8 N 0.23423 0.56363 0.23736
H*9 H 0.21773 0.65942 0.43675
H*10 H 0.27743 0.68302 0.24738
H*11 H 0.37333 0.07817 -0.01189
C1+ C 0.13384 0.38802 0.65602
N'2+ N 0.06007 0.20860 0.48283
C3+ C 0.23837 0.37329 0.65336
C4+ C 0.42428 0.34268 0.63978
N'5+ N -0.02232 0.30250 0.55882
N'6+ N -0.00321 0.53272 0.77159
N7+ N 0.09355 0.58634 0.83185
N'8+ N 0.30202 0.56998 0.77139
N9+ N 0.39666 0.55146 0.76424
N10+ N 0.35291 0.15027 0.52338
N'11+ N 0.25759 0.16264 0.52976
O12+ O 0.13937 0.81375 1.04885
O13+ O 0.38022 -0.03852 0.41169
O14+ O 0.46306 0.72571 0.87070
N15+ N 0.51922 0.32661 0.63284
H*16+ H 0.53650 0.16906 0.53780
H*17+ H 0.56954 0.47183 0.71984
H*18+ H 0.08531 0.90163 1.14038

#END

data_3e_q_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                 11.956
_cell_length_b                 5.252
_cell_length_c                 18.239
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1145.28
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.27872 0.51757 -0.19168
N2 N -0.38182 0.44273 -0.22025
H*3 H -0.44253 0.42258 -0.18182
N'4 N -0.18868 0.40558 -0.21417
N5 N -0.28380 0.71067 -0.14011
H*6 H -0.34634 0.83766 -0.14841
H*7 H -0.20730 0.79136 -0.13242
N8 N -0.08928 0.52628 -0.18486
H*9 H -0.06465 0.42090 -0.14055
H*10 H -0.02878 0.49679 -0.22322
H*11 H -0.37441 0.28558 -0.25223
C1+ C -0.25184 0.73536 0.61674
N'2+ N -0.35902 0.73198 0.59640
C3+ C -0.16066 0.58191 0.58583
C4+ C 0.00060 0.31083 0.52861
N'5+ N -0.41228 0.90323 0.63850
N'6+ N -0.34302 1.01368 0.68417
N7+ N -0.24346 0.91057 0.67068
N'8+ N -0.05734 0.67479 0.59414
N9+ N 0.02404 0.53275 0.56502
N10+ N -0.10871 0.23258 0.52289
N'11+ N -0.19219 0.36729 0.55215
O12+ O -0.15076 0.97860 0.70972
O13+ O -0.12781 0.02810 0.48952
O14+ O 0.12461 0.60037 0.56995
N15+ N 0.08284 0.17177 0.49940
H*16+ H 0.06196 0.00993 0.47267
H*17+ H 0.16215 0.23619 0.50453
H*18+ H -0.18013 1.09015 0.74780

#END

data_3e_q_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 7.967
_cell_length_b 16.552
_cell_length_c 8.433
_cell_angle_alpha 90.00
_cell_angle_beta 98.53
_cell_angle_gamma 90.00
_cell_volume 1099.76
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.20422 0.49592 0.18691
N2 N 0.11441 0.47081 0.30806
H*3 H 0.09075 0.41057 0.30732
N'4 N 0.15621 0.56037 0.10592
N5 N 0.34018 0.44724 0.16487
H*6 H 0.39936 0.42084 0.26640
H*7 H 0.41971 0.47631 0.09993
N8 N 0.27461 0.58207 -0.00189
H*9 H 0.22574 0.56034 -0.11268
H*10 H 0.26613 0.64325 -0.01279
H*11 H 0.00734 0.50389 0.30880
C1+ C 0.34056 -0.18056 -0.09117
N'2+ N 0.21856 -0.23643 -0.11161
C3+ C 0.49393 -0.17825 -0.16845
C4+ C 0.76390 -0.17457 -0.31062
N'5+ N 0.10258 -0.21437 -0.01946
N'6+ N 0.14668 -0.14711 0.05743
N7+ N 0.29388 -0.12588 0.01290
N'8+ N 0.56562 -0.10576 -0.17829
N9+ N 0.70414 -0.10516 -0.25027
N10+ N 0.68032 -0.24606 -0.29476
N'11+ N 0.54296 -0.24933 -0.22161
O12+ O 0.37935 -0.05846 0.07295
O13+ O 0.73814 -0.30879 -0.35054
O14+ O 0.78289 -0.04047 -0.26531
N15+ N 0.90194 -0.17289 -0.38315
H*16+ H 0.94140 -0.22536 -0.42673
H*17+ H 0.95953 -0.11907 -0.39301
H*18+ H 0.31428 -0.03955 0.15476

#END

S46. Optimized crystal structure coordinates for 5 polymorphs of Diaminoguanidine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

```
data_3f_q_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                 18.763
_cell_length_b                 12.585
_cell_length_c                 5.086
_cell_angle_alpha               90.00
_cell_angle_beta                86.79
_cell_angle_gamma                 90.00
_cell_volume                   1199.08
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.08890 -0.26451 0.15662
N'2 N 0.06404 -0.30465 -0.05341
N3 N 0.08351 -0.15532 0.20410
H*4 H 0.12801 -0.12439 0.27873
N5 N 0.12333 -0.32054 0.34744
N6 N 0.05873 -0.08867 0.00368
N7 N 0.06989 -0.41895 -0.05799
H*8 H 0.11936 -0.43793 -0.13954
H*9 H 0.07249 -0.12248 -0.17507
H*10 H 0.00439 -0.09054 0.02078
H*11 H 0.03494 -0.44364 -0.19108
H*12 H 0.11611 -0.28986 0.53135
H*13 H 0.11203 -0.39951 0.33863
C1+ C 0.63581 0.21083 0.57836
N'2+ N 0.65885 0.11143 0.60708
C3+ C 0.66630 0.30744 0.68860
C4+ C 0.72269 0.47841 0.88198
N'5+ N 0.61598 0.04877 0.47183
N'6+ N 0.56725 0.10470 0.35958
N7+ N 0.57952 0.20520 0.42463
N'8+ N 0.65314 0.39837 0.56445
N9+ N 0.68195 0.48499 0.66723
N10+ N 0.73320 0.38082 0.99454
N'11+ N 0.70449 0.29267 0.89995
O12+ O 0.53741 0.28608 0.34439
O13+ O 0.77050 0.37710 1.19166
O14+ O 0.67268 0.57506 0.56794
N15+ N 0.75149 0.56566 0.98140
```

```
H*16+ H 0.78149 0.55731 1.13917
H*17+ H 0.74275 0.63594 0.89245
H*18+ H 0.49899 0.24971 0.25980

#END

data_3f_q_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                 8.936
_cell_length_b                 19.210
_cell_length_c                 6.934
_cell_angle_alpha               90.00
_cell_angle_beta                92.40
_cell_angle_gamma                 90.00
_cell_volume                   1189.25
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.20910 0.06681 0.10995
N'2 N -0.20093 0.00533 0.18531
N3 N -0.07872 0.10550 0.08581
H*4 H -0.09126 0.15664 0.11757
N5 N -0.34009 0.10087 0.05069
N6 N 0.05882 0.07987 0.16699
N7 N -0.34542 -0.02818 0.18531
H*8 H -0.39633 -0.01347 0.30838
H*9 H 0.03672 0.05110 0.28679
H*10 H 0.09943 0.04539 0.07056
H*11 H -0.32313 -0.07979 0.20257
H*12 H -0.32825 0.13380 -0.06194
H*13 H -0.42598 0.06656 0.02945
C1+ C 0.08010 0.81437 0.39637
N'2+ N 0.00524 0.75749 0.33848
C3+ C 0.23473 0.81748 0.47628
C4+ C 0.51144 0.82174 0.61384
N'5+ N -0.13111 0.77873 0.27421
N'6+ N -0.14459 0.84639 0.28917
N7+ N -0.01373 0.86866 0.36433
N'8+ N 0.30510 0.87847 0.45992
N9+ N 0.44602 0.87980 0.53228
```

N10+ N 0.42936 0.76144 0.62288
N'11+ N 0.28761 0.75830 0.55469
O12+ O 0.01137 0.93740 0.40355
O13+ O 0.49179 0.70911 0.69900
O14+ O 0.52276 0.93454 0.52626
N15+ N 0.65275 0.82379 0.68446
H*16+ H 0.69709 0.77973 0.74258
H*17+ H 0.70964 0.86906 0.67446
H*18+ H -0.08615 0.95895 0.37819

#END

data_3f_q_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 15.807
_cell_length_b 10.181
_cell_length_c 4.930
_cell_angle_alpha 53.44
_cell_angle_beta 105.19
_cell_angle_gamma 86.19
_cell_volume 589.127
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.38031 0.17970 -0.37763
N'2 N 0.38874 0.26951 -0.27222
N3 N 0.30316 0.12124 -0.39748
H*4 H 0.31830 0.00023 -0.30814
N5 N 0.44351 0.12969 -0.47150
N6 N 0.24093 0.14377 -0.25740
N7 N 0.46919 0.32812 -0.29488
H*8 H 0.52307 0.23465 -0.05647
H*9 H 0.27644 0.14293 -0.05007
H*10 H 0.19756 0.26404 -0.45766
H*11 H 0.45835 0.42693 -0.29234
H*12 H 0.41536 0.11782 -0.66316
H*13 H 0.48660 0.20432 -0.53326
C1+ C 0.72118 0.30277 0.22345
N'2+ N 0.66581 0.20269 0.30126
C3+ C 0.79954 0.28866 0.12604
C4+ C 0.93735 0.26314 -0.05519
N'5+ N 0.60342 0.26244 0.37060

N'6+ N 0.61732 0.39559 0.33895
N7+ N 0.69010 0.42120 0.24677
N'8+ N 0.82459 0.43094 -0.06417
N9+ N 0.89555 0.41512 -0.15201
N10+ N 0.90603 0.12444 0.13944
N'11+ N 0.83617 0.13447 0.23683
O12+ O 0.72534 0.54948 0.19714
O13+ O 0.94578 -0.01339 0.22586
O14+ O 0.92552 0.54025 -0.32846
N15+ N 1.00786 0.24968 -0.14704
H*16+ H 1.03650 0.13552 -0.07194
H*17+ H 1.02869 0.35478 -0.29146
H*18+ H 0.69007 0.59602 0.27155

#END

data_3f_q_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 10.521
_cell_length_b 9.469
_cell_length_c 12.449
_cell_angle_alpha 90.00
_cell_angle_beta 76.71
_cell_angle_gamma 90.00
_cell_volume 1207
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.19101 0.42833 0.72473
N'2 N 0.15219 0.37702 0.64153
N3 N 0.31500 0.48909 0.70924
H*4 H 0.36071 0.46413 0.77009
N5 N 0.12040 0.42726 0.83363
N6 N 0.40230 0.47727 0.60427
N7 N 0.01875 0.32854 0.67256
H*8 H 0.01972 0.22645 0.69938
H*9 H 0.38153 0.38586 0.56784
H*10 H 0.38021 0.55692 0.55665
H*11 H -0.01149 0.32257 0.60074
H*12 H 0.13923 0.51040 0.87891

H*13 H 0.02345 0.41287 0.83809
C1+ C 0.64801 0.08509 0.26471
N'2+ N 0.54612 0.16012 0.24977
C3+ C 0.73707 -0.00046 0.18175
C4+ C 0.89605 -0.14926 0.03177
N'5+ N 0.49348 0.22248 0.34670
N'6+ N 0.55815 0.18984 0.42146
N7+ N 0.65420 0.10502 0.37082
N'8+ N 0.85555 -0.02422 0.20006
N9+ N 0.93510 -0.10131 0.12295
N10+ N 0.77213 -0.11846 0.02060
N'11+ N 0.68915 -0.04348 0.09659
O12+ O 0.74057 0.04791 0.42538
O13+ O 0.73868 -0.16414 -0.06348
O14+ O 1.04862 -0.13121 0.13190
N15+ N 0.97703 -0.22547 -0.04493
H*16+ H 0.94466 -0.25823 -0.11122
H*17+ H 1.06759 -0.24546 -0.03395
H*18+ H 0.70596 0.07578 0.50184

#END

data_3f_q_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 9.876
_cell_length_b 10.444
_cell_length_c 12.003
_cell_angle_alpha 107.52
_cell_angle_beta 120.65
_cell_angle_gamma 120.11
_cell_volume 611.358
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.18844 -0.00703 -0.11849
N'2 N 0.22750 -0.07559 -0.04881
N3 N 0.19282 -0.03183 -0.23730
H*4 H 0.28403 0.10264 -0.20882
N5 N 0.14530 0.09765 -0.08349
N6 N 0.27275 -0.10678 -0.25911
N7 N 0.19670 -0.05038 0.05804
H*8 H 0.37263 0.10739 0.19891

H*9 H 0.40198 -0.05635 -0.13452
H*10 H 0.11269 -0.27648 -0.36637
H*11 H 0.16910 -0.15367 0.06556
H*12 H 0.02959 0.06762 -0.19527
H*13 H 0.08525 0.06743 -0.03624
C1+ C 0.09500 0.34822 0.74119
N'2+ N -0.03631 0.20506 0.73370
C3+ C 0.23968 0.37412 0.72190
C4+ C 0.49059 0.41307 0.68242
N'5+ N -0.14012 0.23700 0.75605
N'6+ N -0.07972 0.39358 0.77687
N7+ N 0.06538 0.46242 0.76718
N'8+ N 0.27510 0.46330 0.66388
N9+ N 0.40536 0.48338 0.64590
N10+ N 0.44315 0.32274 0.74073
N'11+ N 0.31699 0.30278 0.76306
O12+ O 0.16775 0.62981 0.78715
O13+ O 0.52423 0.26050 0.77396
O14+ O 0.45184 0.56654 0.59364
N15+ N 0.61913 0.43302 0.66260
H*16+ H 0.67755 0.37810 0.69002
H*17+ H 0.64937 0.49956 0.61871
H*18+ H 0.12469 0.68347 0.82196

#END

S47. Optimized crystal structure coordinates for 5 polymorphs of Triaminoguanidine - 6-amino-3-(1-hydroxy-1*H*-tetrazole-5-yl)-1,2,4,5-tetrazine 1,5-dioxide (cocrystal form).

data_3g_q_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 13.029
_cell_length_b 8.681
_cell_length_c 11.496
_cell_angle_alpha 90.00
_cell_angle_beta 108.34
_cell_angle_gamma 90.00
_cell_volume 1234.21
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y

```
_atom_site_fract_z
C1 C 0.47644 0.41197 -0.35551
N'2 N 0.44514 0.30613 -0.43887
N3 N 0.33017 0.27909 -0.47192
N4 N 0.40506 0.49620 -0.31198
N5 N 0.45019 0.58101 -0.20240
N6 N 0.58494 0.44722 -0.30667
N7 N 0.65781 0.39695 -0.36738
H*8 H 0.31746 0.17838 -0.51946
H*9 H 0.29120 0.36162 -0.53375
H*10 H 0.33710 0.43328 -0.31967
H*11 H 0.40364 0.67573 -0.20554
H*12 H 0.45230 0.51705 -0.12727
H*13 H 0.60180 0.55237 -0.26752
H*14 H 0.67268 0.28322 -0.34678
H*15 H 0.61866 0.39928 -0.45983
C1+ C 0.45154 -0.02815 0.24188
N'2+ N 0.35900 -0.10694 0.21329
C3+ C 0.53709 -0.04305 0.18455
C4+ C 0.68697 -0.06931 0.07890
N'5+ N 0.30488 -0.05548 0.28753
N'6+ N 0.35948 0.05216 0.36109
N7+ N 0.45029 0.06967 0.33279
N'8+ N 0.60175 0.07899 0.19390
N9+ N 0.67834 0.06303 0.14013
N10+ N 0.61604 -0.18801 0.07429
N'11+ N 0.53942 -0.17733 0.12833
O12+ O 0.52820 0.17197 0.39380
O13+ O 0.62600 -0.30815 0.01803
O14+ O 0.74434 0.16997 0.14380
N15+ N 0.76356 -0.08312 0.02496
H*16+ H 0.76684 -0.18235 -0.01980
H*17+ H 0.81395 0.00698 0.03000
H*18+ H 0.50269 0.20954 0.45968

#END

data_3g_q_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                 9.859
_cell_length_b                 17.205
_cell_length_c                 7.692
_cell_angle_alpha               90.00
```

```
_cell_angle_beta                 82.56
_cell_angle_gamma                90.00
_cell_volume                   1293.76
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.33101 0.68371 -0.42936
N'2 N 0.27063 0.75059 -0.43262
N3 N 0.36226 0.80956 -0.51330
N4 N 0.46457 0.67048 -0.50769
N5 N 0.52889 0.60140 -0.46014
N6 N 0.26213 0.62110 -0.34745
N7 N 0.11837 0.62431 -0.30621
H*8 H 0.31425 0.86089 -0.48157
H*9 H 0.36638 0.80478 -0.64662
H*10 H 0.52001 0.72066 -0.51153
H*11 H 0.59582 0.58383 -0.56426
H*12 H 0.58068 0.61040 -0.35541
H*13 H 0.29900 0.56815 -0.38595
H*14 H 0.09799 0.65745 -0.19607
H*15 H 0.07979 0.65535 -0.40230
C1+ C -0.08444 0.11189 0.90623
N'2+ N -0.18042 0.08545 0.81396
C3+ C 0.06245 0.09426 0.87624
C4+ C 0.32398 0.06338 0.81734
N'5+ N -0.29947 0.11680 0.88553
N'6+ N -0.28200 0.16174 1.01827
N7+ N -0.14877 0.15900 1.03114
N'8+ N 0.14534 0.14608 0.93777
N9+ N 0.27853 0.12904 0.90756
N10+ N 0.23014 0.01396 0.75901
N'11+ N 0.09612 0.02839 0.78875
O12+ O -0.09390 0.19845 1.15927
O13+ O 0.27448 -0.04591 0.67734
O14+ O 0.36596 0.17330 0.96055
N15+ N 0.45754 0.04741 0.78725
H*16+ H 0.48688 -0.00142 0.71943
H*17+ H 0.52341 0.08535 0.83170
H*18+ H -0.17352 0.21931 1.23267

#END

data_3g_q_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                10.055
_cell_length_b                10.069
_cell_length_c                13.876
_cell_angle_alpha              90.00
_cell_angle_beta               63.97
_cell_angle_gamma                90.00
_cell_volume                  1262.36
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.18968 0.57687 0.64937
N'2 N 0.10273 0.61936 0.60931
N3 N -0.01078 0.70608 0.68292
N4 N 0.17979 0.61964 0.74783
N5 N 0.25629 0.54385 0.79370
N6 N 0.29972 0.48618 0.59333
N7 N 0.34110 0.46499 0.48320
H*8 H -0.08652 0.71413 0.65314
H*9 H 0.03331 0.79918 0.67675
H*10 H 0.07400 0.64782 0.79705
H*11 H 0.28809 0.60586 0.83746
H*12 H 0.19047 0.47108 0.84250
H*13 H 0.38462 0.48262 0.61370
H*14 H 0.26250 0.40517 0.47830
H*15 H 0.33180 0.55328 0.45000
C1+ C 0.10629 0.61314 0.25470
N'2+ N 0.01444 0.69805 0.24064
C3+ C 0.20558 0.51770 0.17601
C4+ C 0.38388 0.35091 0.03352
N'5+ N -0.05341 0.76674 0.33245
N'6+ N -0.00779 0.72860 0.40316
N7+ N 0.09151 0.63367 0.35511
N'8+ N 0.32268 0.47795 0.19009
N9+ N 0.41194 0.39199 0.11695
N10+ N 0.26053 0.39823 0.02613
N'11+ N 0.16755 0.48273 0.09844
O12+ O 0.16072 0.56889 0.40683
O13+ O 0.23712 0.35859 -0.05083
O14+ O 0.52496 0.34704 0.12256
N15+ N 0.47470 0.26556 -0.03933
H*16+ H 0.45045 0.23825 -0.09994
H*17+ H 0.56461 0.23339 -0.03136
H*18+ H 0.11098 0.60223 0.48004

#END
```

```
data_3g_q_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                 8.173
_cell_length_b                 18.850
_cell_length_c                 8.310
_cell_angle_alpha               90.00
_cell_angle_beta                86.17
_cell_angle_gamma               90.00
_cell_volume                   1277.39
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.20520 0.51222 0.59038
N'2 N -0.19561 0.45145 0.66244
N3 N -0.26987 0.39551 0.57362
N4 N -0.26799 0.52010 0.43953
N5 N -0.30730 0.58990 0.39183
N6 N -0.14975 0.57295 0.66214
N7 N -0.04743 0.56699 0.79193
H*8 H -0.28241 0.35412 0.65190
H*9 H -0.18687 0.37895 0.48360
H*10 H -0.35129 0.48111 0.42119
H*11 H -0.29048 0.59291 0.26983
H*12 H -0.42610 0.60222 0.42593
H*13 H -0.12174 0.61389 0.58670
H*14 H -0.12122 0.55500 0.89200
H*15 H 0.02572 0.52328 0.77269
C1+ C 0.11249 0.28859 -0.06231
N'2+ N 0.04475 0.22444 -0.07142
C3+ C 0.27062 0.30574 0.00231
C4+ C 0.55441 0.33458 0.11450
N'5+ N -0.09824 0.23329 -0.13971
N'6+ N -0.12264 0.30014 -0.17385
N7+ N 0.00797 0.33453 -0.12645
N'8+ N 0.34213 0.36589 -0.05072
N9+ N 0.48648 0.38000 0.00883
N10+ N 0.47097 0.27390 0.16099
N'11+ N 0.32542 0.25844 0.10599
O12+ O 0.02245 0.40641 -0.14123
```

O13+ O 0.53565 0.23336 0.25839
O14+ O 0.56438 0.43540 -0.03159
N15+ N 0.69931 0.34922 0.17217
H*16+ H 0.74555 0.31416 0.24925
H*17+ H 0.75720 0.39426 0.13461
H*18+ H -0.08311 0.42108 -0.17791

#END

data_3g_q_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 10.035
_cell_length_b 18.380
_cell_length_c 6.035
_cell_angle_alpha 57.27
_cell_angle_beta 111.24
_cell_angle_gamma 71.95
_cell_volume 666.972
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.47880 0.76562 0.88849
N'2 N 0.48703 0.71738 1.15399
N3 N 0.43445 0.64890 1.19783
N4 N 0.43860 0.74519 0.69172
N5 N 0.39067 0.82178 0.36375
N6 N 0.51308 0.84014 0.79164
N7 N 0.60091 0.84252 1.02813
H*8 H 0.41299 0.63216 1.36606
H*9 H 0.54804 0.57227 1.33031
H*10 H 0.35815 0.72255 0.69897
H*11 H 0.43362 0.77883 0.31466
H*12 H 0.24977 0.88688 0.16540
H*13 H 0.55116 0.85215 0.64893
H*14 H 0.50126 0.88697 1.01494
H*15 H 0.69467 0.76194 1.27864
C1+ C -0.11004 0.35243 0.44966
N'2+ N -0.24590 0.38463 0.45670
C3+ C -0.03856 0.27112 0.44414
C4+ C 0.08299 0.12809 0.42593
N'5+ N -0.26672 0.46056 0.45608
N'6+ N -0.15000 0.47730 0.44843

N7+ N -0.05305 0.41064 0.44344
N'8+ N 0.04496 0.28080 0.31255
N9+ N 0.10738 0.20647 0.30774
N10+ N -0.00552 0.12553 0.55517
N'11+ N -0.06747 0.19729 0.56901
O12+ O 0.08538 0.40489 0.44154
O13+ O -0.02537 0.05261 0.66301
O14+ O 0.18949 0.20706 0.19212
N15+ N 0.14516 0.05482 0.41733
H*16+ H 0.12354 -0.00129 0.50538
H*17+ H 0.20895 0.05966 0.31911
H*18+ H 0.09664 0.45024 0.47180

#END