Enthalpies of formation of some N-oxide bitetrazole salts

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.)

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S66. Optimized crystal structure coordinates for 5 polymorphs of **9e** (ionic form).

S67. Optimized crystal structure coordinates for 5 polymorphs of **9f** (ionic form).

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S69. Optimized crystal structure coordinates for first energy polymorph of **1a** for cocrystal form.

S70. Optimized crystal structure coordinates for first energy polymorph of **1b** for cocrystal form.

S71. Optimized crystal structure coordinates for first energy polymorph of **1c** for cocrystal form.

S72. Optimized crystal structure coordinates for first energy polymorph of **1d** for cocrystal form.

S73. Optimized crystal structure coordinates for first energy polymorph of **1e** for cocrystal form.

S74. Optimized crystal structure coordinates for first energy polymorph of **1f** for cocrystal form.

S75. Optimized crystal structure coordinates for first energy polymorph of **1g** for cocrystal form.

S76. Optimized crystal structure coordinates for first energy polymorph of **2a** for cocrystal form.

S77. Optimized crystal structure coordinates for first energy polymorph of **2b** for cocrystal form.

S78. Optimized crystal structure coordinates for first energy polymorph of **2c** for cocrystal form.

S79. Optimized crystal structure coordinates for first energy polymorph of **2d** for cocrystal form.

S80. Optimized crystal structure coordinates for first energy polymorph of **2e** for cocrystal form.

S81. Optimized crystal structure coordinates for first energy polymorph of **2f** for cocrystal form.

S82. Optimized crystal structure coordinates for first energy polymorph of **2g** for cocrystal form.

S83. Optimized crystal structure coordinates for first energy polymorph of **3a** for cocrystal form.

S84. Optimized crystal structure coordinates for first energy polymorph of **3b** for cocrystal form.

S85. Optimized crystal structure coordinates for first energy polymorph of **3c** for cocrystal form.

S86. Optimized crystal structure coordinates for first energy polymorph of **3d** for cocrystal form.

S87. Optimized crystal structure coordinates for first energy polymorph of **3e** for cocrystal form.

S88. Optimized crystal structure coordinates for first energy polymorph of **3f** for cocrystal form.

S89. Optimized crystal structure coordinates for first energy polymorph of **3g** for cocrystal form.

S90. Optimized crystal structure coordinates for first energy polymorph of **4a** for cocrystal form.

S91. Optimized crystal structure coordinates for first energy polymorph of **4b** for cocrystal form.

S92. Optimized crystal structure coordinates for first energy polymorph of **4c** for cocrystal form.

S93. Optimized crystal structure coordinates for first energy polymorph of **4d** for cocrystal form.

S94. Optimized crystal structure coordinates for first energy polymorph of **4e** for cocrystal form.

S95. Optimized crystal structure coordinates for first energy polymorph of **4f** for cocrystal form.

S96. Optimized crystal structure coordinates for first energy polymorph of **4g** for cocrystal form.

S97. Optimized crystal structure coordinates for first energy polymorph of **5a** for cocrystal form.

S98. Optimized crystal structure coordinates for first energy polymorph of **5b** for cocrystal form.

S99. Optimized crystal structure coordinates for first energy polymorph of **5c** for cocrystal form.

S100. Optimized crystal structure coordinates for first energy polymorph of **5d** for cocrystal form.

S101. Optimized crystal structure coordinates for first energy polymorph of **5e** for cocrystal form.

S102. Optimized crystal structure coordinates for first energy polymorph of **5f** for cocrystal form.

S103. Optimized crystal structure coordinates for first energy polymorph of **5g** for cocrystal form.

S104. Optimized crystal structure coordinates for first energy polymorph of **6a** for cocrystal form.

S105. Optimized crystal structure coordinates for first energy polymorph of **6b** for cocrystal form.

S106. Optimized crystal structure coordinates for first energy polymorph of **6c** for cocrystal form.

S107. Optimized crystal structure coordinates for first energy polymorph of **6d** for cocrystal form.

S108. Optimized crystal structure coordinates for first energy polymorph of **6e** for cocrystal form.

S109. Optimized crystal structure coordinates for first energy polymorph of **6f** for cocrystal form.

S110. Optimized crystal structure coordinates for first energy polymorph of **6g** for cocrystal form.

S111. Optimized crystal structure coordinates for first energy polymorph of **7a** for cocrystal form.

S112. Optimized crystal structure coordinates for first energy polymorph of **7b** for cocrystal form.

S113. Optimized crystal structure coordinates for first energy polymorph of **7c** for cocrystal form.

S114. Optimized crystal structure coordinates for first energy polymorph of **7d** for cocrystal form.

S115. Optimized crystal structure coordinates for first energy polymorph of **7e** for cocrystal form.

S116. Optimized crystal structure coordinates for first energy polymorph of **7f** for cocrystal form.

S117. Optimized crystal structure coordinates for first energy polymorph of **7g** for cocrystal form.

S118. Optimized crystal structure coordinates for first energy polymorph of **8a** for cocrystal form.

S119. Optimized crystal structure coordinates for first energy polymorph of **8b** for cocrystal form.

S120. Optimized crystal structure coordinates for first energy polymorph of **8c** for cocrystal form.

S121. Optimized crystal structure coordinates for first energy polymorph of **8d** for cocrystal form.

S122. Optimized crystal structure coordinates for first energy polymorph of **8e** for cocrystal form.

S123. Optimized crystal structure coordinates for first energy polymorph of **8f** for cocrystal form.

S124. Optimized crystal structure coordinates for first energy polymorph of **8g** for cocrystal form.

S125. Optimized crystal structure coordinates for first energy polymorph of **9a** for cocrystal form.

S126. Optimized crystal structure coordinates for first energy polymorph of **9b** for cocrystal form.

S127. Optimized crystal structure coordinates for first energy polymorph of **9c** for cocrystal form.

S128. Optimized crystal structure coordinates for first energy polymorph of **9d** for cocrystal form.

S129. Optimized crystal structure coordinates for first energy polymorph of **9e** for cocrystal form.

S130. Optimized crystal structure coordinates for first energy polymorph of **9f** for cocrystal form.

S131. Optimized crystal structure coordinates for first energy polymorph of **9g** for cocrystal form.

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

Ionic compounds

1

N	1.29494100	2.49397500	0.00000000
N	-0.78667600	1.77804800	0.00000000
N	0.04799400	2.85409900	0.00000000
N	1.27954900	1.14441200	0.00000000
C	0.00000000	0.70152700	0.00000000
C	-0.29163600	-0.71763300	0.00000000
N	0.71955000	-1.61329300	0.00000000
N	0.10570800	-2.79988800	0.00000000
N	-1.21501700	-2.61735700	0.00000000
N	-1.49812000	-1.30798900	0.00000000
H	2.11431100	0.57259600	0.00000000

2

N	-0.41329100	2.70437400	0.00000000
N	1.19540200	1.26307000	0.00000000
N	0.90869900	2.59071300	0.00000000
N	-1.00167500	1.51296800	0.00000000
C	0.00000000	0.60501800	0.00000000
C	-0.25842900	-0.80736300	0.00000000
N	-1.53939500	-1.25589500	0.00000000
N	-1.54441300	-2.60598500	0.00000000
N	-0.29598700	-2.95812900	0.00000000
N	0.53563300	-1.88040300	0.00000000
O	2.37708100	0.78923700	0.00000000
H	-2.38089000	-0.69482100	0.00000000

3

N	0.71563100	2.47369400	0.00000000
N	1.34831000	0.32431600	0.00000000
N	1.75659200	1.59851800	0.00000000
N	-0.39910200	1.74420200	0.00000000
C	0.00000000	0.46651600	0.00000000
C	-0.84339000	-0.70782400	0.00000000
N	-2.16979700	-0.84740500	0.00000000
N	-2.40506600	-2.18707000	0.00000000
N	-1.30183300	-2.87000900	0.00000000
N	-0.30942100	-1.95264400	0.00000000
O	2.96759100	1.95736900	0.00000000
H	0.67241300	-2.19631000	0.00000000

4

N	1.14553000	-2.70279300	0.00000000
N	-0.66072400	-1.63686100	0.00000000
N	-0.15510000	-2.86696700	0.00000000
N	1.48715700	-1.39303700	0.00000000
C	0.33776000	-0.71173700	0.00000000

C	0.00000000	0.68658500	0.00000000
N	0.78561500	1.79602900	0.00000000
N	-0.05701000	2.87154600	0.00000000
N	-1.29310800	2.40922700	0.00000000
N	-1.29452400	1.07968400	0.00000000
O	-2.01029600	-1.42982400	0.00000000
O	2.05358300	1.88828200	0.00000000
H	-2.07769400	-0.41455700	0.00000000

5

N	0.64560200	-2.80915200	0.00000000
N	-1.17914300	-1.50043200	0.00000000
N	-0.71186600	-2.75564000	0.00000000
N	1.07286700	-1.54819100	0.00000000
C	-0.03177300	-0.78452800	0.00000000
C	0.00000000	0.66582700	0.00000000
N	1.14755100	1.39206200	0.00000000
N	0.65224400	2.60270800	0.00000000
N	-0.65755700	2.71913100	0.00000000
N	-1.10281100	1.46993700	0.00000000
O	-1.44561300	-3.78721100	0.00000000
O	1.47940000	3.69712900	0.00000000
H	0.85213000	4.43989600	0.00000000

6

N	-1.77540900	1.75753900	0.00000000
N	0.48186600	1.79168600	0.00000000
N	-0.65868800	2.51836300	0.00000000
N	-1.34469500	0.49349700	0.00000000
C	0.00000000	0.53994600	0.00000000
C	0.73411900	-0.70924200	0.00000000
N	0.06872800	-1.89248700	0.00000000
N	0.92675500	-2.90950000	0.00000000
N	2.11527300	-2.35512700	0.00000000
N	2.03579900	-1.00438000	0.00000000
O	-0.68492700	3.77553700	0.00000000
O	-1.27814400	-2.10385200	0.00000000
H	-1.64755500	-1.15483500	0.00000000

7

N	0.00000000	0.66459700	2.77059100
N	0.00000000	-1.11576300	1.50266500
N	0.00000000	-0.66459700	2.77059100
N	0.00000000	1.11576300	1.50266500
C	0.00000000	0.00000000	0.73753200
C	0.00000000	0.00000000	-0.73753200
N	0.00000000	1.11576300	-1.50266500
N	0.00000000	0.66459700	-2.77059100
N	0.00000000	-0.66459700	-2.77059100
N	0.00000000	-1.11576300	-1.50266500

8

N	0.05896100	2.77544300	0.00000000
N	1.31048500	1.02212700	0.00000000
N	1.32246100	2.37988900	0.00000000
N	-0.77200800	1.72693600	0.00000000
C	0.00000000	0.61770800	0.00000000
C	-0.51385200	-0.75427700	0.00000000
N	-1.84258000	-1.02617600	0.00000000
N	-1.91511200	-2.36567500	0.00000000
N	-0.68819300	-2.88037300	0.00000000
N	0.22064700	-1.88909600	0.00000000
O	2.40256000	0.32723600	0.00000000

9

N	0.14557500	2.51694800	0.00000000
N	1.33227300	0.62444600	0.00000000
N	1.36434100	1.96476300	0.00000000
N	-0.73356300	1.49808900	0.00000000
C	0.00000000	0.36808200	0.00000000
C	-0.56737300	-0.98998400	0.00000000
N	-1.89160600	-1.26082600	0.00000000
N	-1.96427300	-2.60326800	0.00000000
N	-0.73824700	-3.11795100	0.00000000
N	0.16768500	-2.12392200	0.00000000
O	2.45361700	2.65543400	0.00000000

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

Neutral compounds

1Q, 7Q

N	-0.37306100	2.85430200	0.00000000
N	1.23919700	1.37024700	0.00000000
N	0.91292000	2.68946900	0.00000000
N	-0.91292000	1.61972100	0.00000000
C	0.08805400	0.71688700	0.00000000
C	-0.08805400	-0.71688700	0.00000000
N	-1.23919700	-1.37024700	0.00000000
N	-0.91292000	-2.68946900	0.00000000
N	0.37306100	-2.85430200	0.00000000
N	0.91292000	-1.61972100	0.00000000
H	-1.91524900	1.46983900	0.00000000
H	1.91524900	-1.46983900	0.00000000

2Q, 8Q

N	0.53058900	2.77774500	0.00000000
N	1.34612800	0.84006600	0.00000000
N	1.67099200	2.12505600	0.00000000
N	-0.52045100	1.93324900	0.00000000
C	0.00000000	0.71057400	0.00000000
C	-0.64398400	-0.57531200	0.00000000
N	-1.95902800	-0.85255300	0.00000000
N	-2.11161100	-2.19815700	0.00000000
N	-0.92364800	-2.70469300	0.00000000
N	0.01879800	-1.72489800	0.00000000
O	2.30653800	-0.12279300	0.00000000
H	1.80304400	-0.97624700	0.00000000
H	-2.75381800	-0.22369300	0.00000000

3Q

N	0.65190600	2.42931200	0.00000000
N	1.34573800	0.30496000	0.00000000
N	1.65931400	1.57333000	0.00000000
N	-0.43432800	1.67894300	0.00000000
C	0.00000000	0.39823100	0.00000000
C	-0.84308700	-0.78410300	0.00000000
N	-2.16498000	-0.85029100	0.00000000

N	-2.46724000	-2.17504200	0.00000000
N	-1.39639100	-2.90621800	0.00000000
N	-0.35864600	-2.04612500	0.00000000
O	2.96134700	1.96112200	0.00000000
H	0.60048800	-2.37040700	0.00000000
H	2.91964800	2.93457100	0.00000000

4Q

N	-0.60095500	2.76942800	0.00000000
N	1.07965800	1.49887800	0.00000000
N	0.70778500	2.77878700	0.00000000
N	-1.07965800	1.50511000	0.00000000
C	-0.01112100	0.71479100	0.00000000
C	0.01112100	-0.71479100	0.00000000
N	-1.07965800	-1.49887800	0.00000000
N	-0.70778500	-2.77878700	0.00000000
N	0.60095500	-2.76942800	0.00000000
N	1.07965800	-1.50511000	0.00000000
O	2.39468500	1.14642000	0.00000000
O	-2.39468500	-1.14642000	0.00000000
H	2.39750300	0.16090200	0.00000000
H	-2.39750300	-0.16090200	0.00000000

5Q

N	-0.71602800	2.74288600	0.00000000
N	1.12420900	1.46809600	0.00000000
N	0.60334800	2.66565900	0.00000000
N	-1.12420900	1.48639600	0.00000000
C	-0.00257500	0.72831600	0.00000000
C	0.00257500	-0.72831600	0.00000000
N	-1.12420900	-1.46809600	0.00000000
N	-0.60334800	-2.66565900	0.00000000
N	0.71602800	-2.74288600	0.00000000
N	1.12420900	-1.48639600	0.00000000
O	1.40455500	3.76407500	0.00000000
O	-1.40455500	-3.76407500	0.00000000
H	0.78011100	4.51138300	0.00000000
H	-0.78011100	-4.51138300	0.00000000

6Q

N	-1.61343100	1.90768600	0.00000000
N	0.61971200	1.67228800	0.00000000
N	-0.43084000	2.46967600	0.00000000
N	-1.34863700	0.60947400	0.00000000
C	0.00000000	0.48162400	0.00000000
C	0.62406700	-0.82232600	0.00000000
N	-0.10149900	-1.96726400	0.00000000
N	0.71026400	-3.01529900	0.00000000
N	1.92474900	-2.51719800	0.00000000
N	1.90732900	-1.16940100	0.00000000
O	-0.32524500	3.82023700	0.00000000
O	-1.45283200	-2.14987000	0.00000000

H	0.63426100	3.98726000	0.00000000
H	-1.82757800	-1.23571700	0.00000000

9Q

N	0.17959700	2.49346300	0.00000000
N	1.33148800	0.57427100	0.00000000
N	1.35035700	1.87974300	0.00000000
N	-0.70958200	1.51677300	0.00000000
C	0.00000000	0.36362600	0.00000000
C	-0.59455700	-0.96692000	0.00000000
N	0.12851900	-2.12466900	0.00000000
N	-0.74289100	-3.09898900	0.00000000
N	-1.93652000	-2.51333000	0.00000000
N	-1.91070700	-1.18879900	0.00000000
O	2.53300600	2.55065200	0.00000000
H	2.27183100	3.48883500	0.00000000
H	-2.80035700	-3.04353600	0.00000000

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

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 of the gas-phase species M were computed according to the atomization energy method (G3B3):

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

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

	H°(Atoms, 298)	$\Delta H_f°$(Atoms, 298) G3B3
H	52.1	-0.49872823
C	171.3	-37.8259642
N	113	-54.56280323
O	59.6	-75.02973288

Table **S4.** 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.

S5. Optimized crystal structure coordinates for 5 polymorphs of **1a** (ionic form).

```
data_NH4_BTO_0H_1
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P 1'
_symmetry_Int_Tables_number      1
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
_cell_length_a                 16.920
_cell_length_b                 4.618
_cell_length_c                 6.858
_cell_angle_alpha               130.57
_cell_angle_beta                42.05
_cell_angle_gamma                93.67
_cell_volume                   154.699
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.16498 0.71887 0.12654
H*2 H 0.23481 0.39209 -0.25838
H*3 H 0.09312 1.15172 0.39644
H*4 H 0.05640 0.83270 0.43922
H*5 H 0.27559 0.49896 -0.07112
N'1+ N -0.54937 1.20913 1.65933
```

N'2+ N -0.39601 0.97104 1.54757
N'3+ N -0.54353 1.44729 1.89055
N4+ N -0.40167 0.55859 1.15049
C5+ C -0.30709 0.41089 1.08073
C6+ C -0.14181 -0.25898 0.56666
N'7+ N -0.08074 -0.74343 0.15104
N'8+ N 0.07085 -1.28443 -0.25055
N'9+ N 0.09873 -1.12817 -0.08082
N'10+ N -0.03379 -0.48163 0.43560
H*11+ H -0.36953 0.23954 0.87071

#END

data_NH4_BTO_0H_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z
_cell_length_a 13.125
_cell_length_b 10.070
_cell_length_c 10.393
_cell_angle_alpha 90.00
_cell_angle_beta 103.88
_cell_angle_gamma 90.00
_cell_volume 1333.52
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.04428 0.22207 -0.08487
H*2 H -0.10262 0.21741 -0.17069
H*3 H -0.02020 0.31886 -0.06693
H*4 H -0.07246 0.18729 -0.00708
H*5 H 0.01816 0.16470 -0.09479
N'1+ N 0.09781 0.42893 0.41385
N'2+ N 0.13191 0.61531 0.32170
N'3+ N 0.07392 0.55380 0.39667
N4+ N 0.17357 0.40777 0.34837
C5+ C 0.19469 0.52229 0.29160
C6+ C 0.27355 0.52630 0.21512

```
N'7+ N 0.32683 0.41491 0.19995
N'8+ N 0.39168 0.45352 0.12576
N'9+ N 0.37755 0.58245 0.09799
N'10+ N 0.30317 0.63138 0.15326
H*11+ H 0.20814 0.31863 0.34393

#END

data_NH4_BTO_0H_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                 18.727
_cell_length_b                 10.214
_cell_length_c                 4.798
_cell_angle_alpha               90.00
_cell_angle_beta               136.82
_cell_angle_gamma                90.00
_cell_volume                   628.009
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.19610 0.01063 1.22339
H*2 H -0.26585 -0.01991 1.10830
H*3 H -0.16500 -0.06302 1.19190
H*4 H -0.20840 0.09202 1.06678
H*5 H -0.14517 0.03343 1.52659
N'1+ N -0.12780 0.68119 0.06357
N'2+ N -0.05074 0.85644 0.11268
N'3+ N -0.12100 0.80776 0.09878
N4+ N -0.06017 0.64570 0.05406
C5+ C -0.01267 0.75335 0.08422
C6+ C 0.06392 0.74181 0.08141
N'7+ N 0.08851 0.62266 0.04842
N'8+ N 0.15990 0.64764 0.05573
N'9+ N 0.17702 0.77626 0.09156
N'10+ N 0.11733 0.83859 0.10858
H*11+ H -0.04822 0.55192 0.02805

#END

data_NH4_BTO_0H_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                  10.895
_cell_length_b                  8.004
_cell_length_c                  8.138
_cell_angle_alpha               146.22
_cell_angle_beta                91.19
_cell_angle_gamma               109.56
_cell_volume                    305.292
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.32110 0.16091 0.94355
H*2 H 0.29267 0.27224 0.94510
H*3 H 0.21935 -0.09900 0.76962
H*4 H 0.39572 0.11751 0.86106
H*5 H 0.37666 0.35289 1.19840
N'1+ N 0.00331 1.12922 0.32040
N'2+ N 0.24191 1.39902 0.45232
N'3+ N 0.11774 1.40223 0.45379
N4+ N 0.05364 0.94144 0.22875
C5+ C 0.20041 1.10688 0.30965
C6+ C 0.28148 0.95849 0.23726
N'7+ N 0.21050 0.65188 0.08750
N'8+ N 0.31610 0.59373 0.05919
N'9+ N 0.44447 0.85480 0.18677
N'10+ N 0.42610 1.09009 0.30164
H*11+ H -0.01101 0.71199 0.11667

#END

data_NH4_BTO_0H_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                  14.843
```

_cell_length_b 9.103
_cell_length_c 5.228
_cell_angle_alpha 90.00
_cell_angle_beta 67.05
_cell_angle_gamma 90.00
_cell_volume 650.472
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.16773 -0.45446 0.10643
H*2 H 0.13456 -0.39284 0.28320
H*3 H 0.11610 -0.51762 0.07225
H*4 H 0.20070 -0.38583 -0.06021
H*5 H 0.21957 -0.52157 0.13050
N'1+ N 0.02768 0.31008 0.77123
N'2+ N 0.13305 0.20453 0.91463
N'3+ N 0.08339 0.32927 0.90782
N4+ N 0.04109 0.16887 0.68593
C5+ C 0.10589 0.10369 0.77390
C6+ C 0.13305 -0.04887 0.70926
N'7+ N 0.09354 -0.12749 0.55972
N'8+ N 0.13378 -0.26052 0.53934
N'9+ N 0.19466 -0.26097 0.67123
N'10+ N 0.19577 -0.12837 0.78110
H*11+ H 0.00690 0.12147 0.57325

#END

S6. Optimized crystal structure coordinates for 5 polymorphs of **1b** (ionic form).

data_NH3OH_BTO_0H_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a 4.289
_cell_length_b 19.993
_cell_length_c 9.286
_cell_angle_alpha 90.00
_cell_angle_beta 122.28
_cell_angle_gamma 90.00
_cell_volume 673.209
loop_
_atom_site_label
_atom_site_type_symbol

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.38383 0.60068 -0.26197
H*2 H 0.24233 0.62096 -0.38268
H*3 H 0.48886 0.55476 -0.26633
H*4 H 0.59349 0.63294 -0.18117
O5 O 0.11809 0.59446 -0.21811
H*6 H 0.24167 0.57530 -0.10377
N'1+ N -0.32058 -0.26274 0.78016
N'2+ N -0.05826 -0.17339 0.93810
N'3+ N -0.22906 -0.23287 0.92158
N4+ N -0.20684 -0.22178 0.70157
C5+ C -0.04536 -0.16677 0.79849
C6+ C 0.10107 -0.11471 0.74237
N'7+ N 0.07706 -0.12084 0.59188
N'8+ N 0.23554 -0.06524 0.58058
N'9+ N 0.34902 -0.02764 0.71857
N'10+ N 0.26770 -0.05766 0.82351
H*11+ H -0.24060 -0.23186 0.58728

#END

data_NH3OH_BTO_0H_2
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_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
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_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,z
3 x,1/2-y,1/2+z
4 1/2-x,-y,1/2+z
5 -x,-y,-z
6 1/2+x,1/2-y,-z
7 -x,1/2+y,1/2-z
8 1/2+x,y,1/2-z
_cell_length_a                 19.290
_cell_length_b                 9.350
_cell_length_c                 7.611
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   1372.73
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.10238 0.37897 0.32542
```

H*2 H -0.11870 0.46655 0.39651
H*3 H -0.14114 0.34993 0.23884
H*4 H -0.05758 0.40553 0.25861
O5 O -0.09041 0.27251 0.45228
H*6 H -0.07476 0.18709 0.38997
N'1+ N 0.76355 0.16661 0.66940
N'2+ N 0.67336 0.07529 0.53222
N'3+ N 0.73307 0.04901 0.62205
N4+ N 0.72276 0.27309 0.60904
C5+ C 0.66724 0.21718 0.52459
C6+ C 0.61524 0.30953 0.44715
N'7+ N 0.62193 0.45301 0.45889
N'8+ N 0.56622 0.50385 0.37537
N'9+ N 0.52801 0.39515 0.31644
N'10+ N 0.55773 0.27058 0.35989
H*11+ H 0.73329 0.37819 0.62613

#END

data_NH3OH_BTO_0H_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 11.887
_cell_length_b 10.428
_cell_length_c 8.768
_cell_angle_alpha 71.82
_cell_angle_beta 152.83
_cell_angle_gamma 126.72
_cell_volume 317.995
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.39573 0.27091 0.20781
H*2 H 0.37145 0.18037 0.13867
H*3 H 0.62499 0.34992 0.52191
H*4 H 0.41688 0.36707 0.13437
O5 O 0.07336 0.13777 -0.04448
H*6 H 0.08544 0.21806 0.01186
N'1+ N 0.50073 0.31425 -0.01166
N'2+ N 0.73110 0.46438 -0.01233
N'3+ N 0.61598 0.46050 -0.01015
N4+ N 0.54120 0.21941 -0.01493
C5+ C 0.68288 0.31150 -0.01535

```
C6+ C 0.75319 0.23840 -0.01865
N'7+ N 0.67714 0.07671 -0.02135
N'8+ N 0.77320 0.05136 -0.02391
N'9+ N 0.90100 0.19207 -0.02279
N'10+ N 0.89176 0.31289 -0.01947
H*11+ H 0.47359 0.09790 -0.01675

#END

data_NH3OH_BTO_0H_4
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_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
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2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z
_cell_length_a                 13.673
_cell_length_b                 10.029
_cell_length_c                 10.377
_cell_angle_alpha               90.00
_cell_angle_beta                69.19
_cell_angle_gamma                 90.00
_cell_volume                   1330.13
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.05632 -0.71740 0.06017
H*2 H -0.08661 -0.72227 -0.01758
H*3 H -0.11491 -0.68841 0.15018
H*4 H -0.02748 -0.81011 0.07157
O5 O 0.02366 -0.62149 0.01493
H*6 H 0.05463 -0.61377 0.08615
N'1+ N -0.39977 0.46133 0.07840
N'2+ N -0.37043 0.65050 0.16600
N'3+ N -0.42392 0.58688 0.09564
N4+ N -0.32846 0.44188 0.13908
C5+ C -0.31027 0.55812 0.19305
C6+ C -0.23640 0.56417 0.26421
N'7+ N -0.18489 0.45300 0.27719
N'8+ N -0.12464 0.49366 0.34658
N'9+ N -0.13970 0.62356 0.37373
```

N'10+ N -0.21011 0.67110 0.32282
H*11+ H -0.29479 0.35270 0.14230

#END

data_NH3OH_BTO_0H_5
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 8.505
_cell_length_b 8.424
_cell_length_c 5.347
_cell_angle_alpha 103.91
_cell_angle_beta 106.66
_cell_angle_gamma 98.32
_cell_volume 346.721
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.70248 0.35573 0.32171
H*2 H 0.61514 0.25302 0.30911
H*3 H 0.75398 0.42971 0.52301
H*4 H 0.79464 0.31419 0.25074
O5 O 0.60973 0.43901 0.15388
H*6 H 0.68835 0.53782 0.16013
N'1+ N -0.36246 -0.18580 0.49805
N'2+ N -0.33093 0.00705 0.87992
N'3+ N -0.42758 -0.13855 0.68764
N4+ N -0.21910 -0.06806 0.56760
C5+ C -0.19942 0.05073 0.80246
C6+ C -0.05458 0.19186 0.92142
N'7+ N 0.06249 0.20577 0.79764
N'8+ N 0.17565 0.34705 0.95866
N'9+ N 0.12786 0.41431 1.16934
N'10+ N -0.01763 0.31882 1.15145
H*11+ H -0.14030 -0.07107 0.45709

#END

S7. Optimized crystal structure coordinates for 5 polymorphs of **1c** (ionic form).

data_N2H5_BTO_0H_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_

```
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a                 7.951
_cell_length_b                 9.150
_cell_length_c                 9.379
_cell_angle_alpha               90.00
_cell_angle_beta                97.98
_cell_angle_gamma                 90.00
_cell_volume                   675.73
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.42556 -0.20553 -0.18821
H*2 H 0.47772 -0.30389 -0.15201
H*3 H 0.36211 -0.22388 -0.28986
N4 N 0.56296 -0.10434 -0.20012
H*5 H 0.51019 -0.00751 -0.23764
H*6 H 0.62645 -0.08798 -0.09900
H*7 H 0.33879 -0.17359 -0.12196
N'1+ N -0.27124 0.25454 0.47359
N'2+ N -0.10767 0.36948 0.64665
N'3+ N -0.22500 0.38158 0.52682
N4+ N -0.18185 0.15625 0.56080
C5+ C -0.08113 0.22669 0.66736
C6+ C 0.02829 0.14553 0.77592
N'7+ N 0.03040 -0.00202 0.77134
N'8+ N 0.14261 -0.04006 0.88473
N'9+ N 0.20463 0.07983 0.95382
N'10+ N 0.13460 0.19921 0.88743
H*11+ H -0.19111 0.04681 0.54631

#END

data_N2H5_BTO_0H_2
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P 21 21 21'
_symmetry_Int_Tables_number      19
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2+x,1/2-y,-z
3 -x,1/2+y,1/2-z
4 1/2-x,-y,1/2+z
_cell_length_a                 11.660
```

```
_cell_length_b                 9.241
_cell_length_c                 6.444
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   694.341
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.34525 0.10916 0.63769
H*2 H 0.36476 0.00169 0.65968
H*3 H 0.41561 0.16731 0.68589
N4 N 0.24989 0.14545 0.77192
H*5 H 0.23191 0.25265 0.75089
H*6 H 0.18077 0.08608 0.72453
H*7 H 0.33296 0.12722 0.48111
N'1+ N 0.47202 -0.02185 0.25003
N'2+ N 0.63947 0.08813 0.24533
N'3+ N 0.52327 0.10282 0.24881
N4+ N 0.55684 -0.12122 0.24728
C5+ C 0.65995 -0.05383 0.24439
C6+ C 0.76541 -0.13670 0.24106
N'7+ N 0.76138 -0.28279 0.24084
N'8+ N 0.87141 -0.32306 0.23748
N'9+ N 0.93806 -0.20582 0.23579
N'10+ N 0.87337 -0.08603 0.23799
H*11+ H 0.54310 -0.22933 0.24743

#END

data_N2H5_BTO_0H_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                 13.256
_cell_length_b                 9.200
_cell_length_c                 6.522
_cell_angle_alpha               90.00
_cell_angle_beta                118.71
_cell_angle_gamma                 90.00
_cell_volume                   697.608
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.59912 0.38089 0.26622
H*2 H 0.66780 0.32106 0.38585
H*3 H 0.62376 0.48822 0.29545
N4 N 0.50440 0.36120 0.31522
H*5 H 0.43702 0.42220 0.19742
H*6 H 0.48131 0.25409 0.28834
H*7 H 0.58331 0.35276 0.10009
N'1+ N 0.22167 -0.01373 -0.02404
N'2+ N 0.39091 0.09181 0.16834
N'3+ N 0.27457 0.10891 0.05567
N4+ N 0.30554 -0.11418 0.03792
C5+ C 0.40974 -0.04951 0.15630
C6+ C 0.51450 -0.13405 0.24265
N'7+ N 0.50870 -0.27895 0.20519
N'8+ N 0.61855 -0.32129 0.30585
N'9+ N 0.68680 -0.20637 0.39923
N'10+ N 0.62337 -0.08609 0.36205
H*11+ H 0.29045 -0.22118 -0.00054

#END

data_N2H5_BTO_0H_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                 7.106
_cell_length_b                 11.402
_cell_length_c                 9.306
_cell_angle_alpha               90.00
_cell_angle_beta                113.45
_cell_angle_gamma                90.00
_cell_volume                   691.722
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.14765 0.82100 0.38742
H*2 H 0.11066 0.77554 0.46807
```

H*3 H 0.10662 0.90691 0.39256
N4 N 0.02292 0.77593 0.23320
H*5 H 0.05889 0.82238 0.15370
H*6 H 0.06296 0.69026 0.22964
H*7 H 0.30448 0.81696 0.42016
N'1+ N 0.53574 -0.03015 -0.34860
N'2+ N 0.55010 0.14241 -0.44981
N'3+ N 0.54329 0.02386 -0.46896
N4+ N 0.53763 0.05522 -0.24758
C5+ C 0.54646 0.16147 -0.30958
C6+ C 0.55023 0.26816 -0.22391
N'7+ N 0.54491 0.26212 -0.08061
N'8+ N 0.55044 0.37404 -0.03661
N'9+ N 0.55870 0.44369 -0.14903
N'10+ N 0.55878 0.37915 -0.26930
H*11+ H 0.53302 0.03976 -0.14197

#END

data_N2H5_BTO_0H_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 9.631
_cell_length_b 9.332
_cell_length_c 7.932
_cell_angle_alpha 90.00
_cell_angle_beta 74.68
_cell_angle_gamma 90.00
_cell_volume 687.568
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.68996 0.59129 0.19958
H*2 H 0.79212 0.57032 0.21035
H*3 H 0.65946 0.50401 0.13869
N4 N 0.69734 0.71445 0.08651
H*5 H 0.59582 0.73357 0.07492
H*6 H 0.72924 0.80026 0.14699
H*7 H 0.62140 0.60028 0.32354
N'1+ N -0.02903 -0.04581 0.73727
N'2+ N 0.14681 0.06645 0.81190

N'3+ N 0.02586 0.07857 0.75474
N4+ N 0.05823 -0.14232 0.78423
C5+ C 0.16650 -0.07351 0.83020
C6+ C 0.27547 -0.15328 0.88619
N'7+ N 0.26956 -0.29785 0.89286
N'8+ N 0.38379 -0.33538 0.94855
N'9+ N 0.45463 -0.21804 0.97391
N'10+ N 0.38860 -0.10091 0.93550
H*11+ H 0.04264 -0.24953 0.78396

#END

S8. Optimized crystal structure coordinates for 5 polymorphs of **1d** (ionic form).

data_GH_BTO_0H_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 12.462
_cell_length_b 9.508
_cell_length_c 4.269
_cell_angle_alpha 98.16
_cell_angle_beta 72.65
_cell_angle_gamma 121.84
_cell_volume 410.088
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.31103 0.20657 -0.43422
N2 N 0.18793 0.15224 -0.43549
H*3 H 0.14255 0.05973 -0.58317
H*4 H 0.13670 0.20211 -0.28881
N5 N 0.37651 0.13826 -0.63095
H*6 H 0.46959 0.17744 -0.63386
H*7 H 0.33482 0.04548 -0.78247
N8 N 0.36866 0.32920 -0.23620
H*9 H 0.32096 0.38254 -0.08562
H*10 H 0.46158 0.37212 -0.23137
N'1+ N 0.00493 0.77864 1.03545
N'2+ N 0.21156 0.87126 1.00079
N'3+ N 0.10532 0.88755 1.14225
N4+ N 0.04631 0.68830 0.81786
C5+ C 0.17341 0.74505 0.79610
C6+ C 0.24146 0.66872 0.57802
N'7+ N 0.17794 0.53954 0.39382
N'8+ N 0.26779 0.50080 0.22589

N'9+ N 0.38002 0.60269 0.30685
N'10+ N 0.36642 0.71054 0.52957
H*11+ H -0.01109 0.59300 0.69289

#END

data_GH_BTO_0H_2
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 11.912
_cell_length_b 8.549
_cell_length_c 4.563
_cell_angle_alpha 95.96
_cell_angle_beta 102.48
_cell_angle_gamma 111.98
_cell_volume 411.871
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.30807 -0.29734 -0.11507
N2 N 0.37354 -0.36753 -0.24376
H*3 H 0.33176 -0.45873 -0.43875
H*4 H 0.46672 -0.33142 -0.14978
N5 N 0.18483 -0.34761 -0.24449
H*6 H 0.13359 -0.29626 -0.15107
H*7 H 0.13935 -0.43842 -0.43950
N8 N 0.36582 -0.17687 0.14304
H*9 H 0.45885 -0.13702 0.24460
H*10 H 0.31813 -0.12217 0.24406
N'1+ N 0.00312 0.27673 1.04055
N'2+ N 0.20949 0.37423 1.20975
N'3+ N 0.10284 0.38779 1.24672
N4+ N 0.04536 0.18774 0.86322
C5+ C 0.17230 0.24749 0.96685
C6+ C 0.24116 0.17313 0.81534
N'7+ N 0.17858 0.04279 0.56796
N'8+ N 0.26898 0.00645 0.48826
N'9+ N 0.38063 0.11080 0.68021
N'10+ N 0.36609 0.21794 0.89010
H*11+ H -0.01138 0.09132 0.68126

#END

```
data_GH_BTO_0H_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                  11.748
_cell_length_b                  4.636
_cell_length_c                  10.053
_cell_angle_alpha                98.81
_cell_angle_beta                130.05
_cell_angle_gamma                90.01
_cell_volume                    410.633
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.60693 0.62827 -0.19206
N2 N 0.54090 0.75105 -0.13198
H*3 H 0.44072 0.65944 -0.17761
H*4 H 0.58925 0.93903 -0.03919
N5 N 0.54035 0.37941 -0.31492
H*6 H 0.58829 0.28297 -0.36213
H*7 H 0.44017 0.28051 -0.36414
N8 N 0.73954 0.75436 -0.12929
H*9 H 0.79178 0.94240 -0.03645
H*10 H 0.79138 0.66528 -0.17286
N'1+ N -0.27141 0.00387 0.50594
N'2+ N -0.15802 0.41091 0.71027
N'3+ N -0.27970 0.20011 0.60545
N4+ N -0.14072 0.08797 0.54645
C5+ C -0.07075 0.33835 0.67213
C6+ C 0.07253 0.47493 0.73902
N'7+ N 0.13756 0.35221 0.67584
N'8+ N 0.26522 0.53109 0.76440
N'9+ N 0.27565 0.75093 0.87556
N'10+ N 0.15519 0.72143 0.86254
H*11+ H -0.10323 -0.02344 0.48943

#END

data_GH_BTO_0H_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                22.542
_cell_length_b                10.846
_cell_length_c                4.855
_cell_angle_alpha              90.00
_cell_angle_beta               41.48
_cell_angle_gamma                90.00
_cell_volume                  786.221
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.17248 0.07282 0.97153
N2 N -0.19193 -0.04431 0.97734
H*3 H -0.16499 -0.11506 0.99076
H*4 H -0.23414 -0.06549 0.96847
N5 N -0.11639 0.09815 0.98358
H*6 H -0.10079 0.18599 0.97948
H*7 H -0.08797 0.03019 0.99712
N8 N -0.20913 0.16463 0.95369
H*9 H -0.25167 0.14754 0.94435
H*10 H -0.19534 0.25377 0.94901
N'1+ N 0.50815 0.29623 -0.02854
N'2+ N 0.60619 0.29143 -0.03109
N'3+ N 0.55701 0.36267 -0.03461
N4+ N 0.52569 0.17810 -0.02082
C5+ C 0.58599 0.17490 -0.02237
C6+ C 0.61622 0.05836 -0.01514
N'7+ N 0.58414 -0.04855 -0.00674
N'8+ N 0.62525 -0.13566 -0.00187
N'9+ N 0.67949 -0.08276 -0.00716
N'10+ N 0.67523 0.04017 -0.01561
H*11+ H 0.49712 0.10456 -0.01485

#END

data_GH_BTO_0H_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                9.252
```

_cell_length_b 4.559
_cell_length_c 13.170
_cell_angle_alpha 118.53
_cell_angle_beta 82.98
_cell_angle_gamma 66.28
_cell_volume 411.287
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.79770 -0.06773 -0.19249
N2 N 0.67742 -0.09027 -0.13465
H*3 H 0.63785 0.03320 -0.04147
H*4 H 0.62260 -0.23143 -0.18244
N5 N 0.86806 0.12098 -0.12688
H*6 H 0.95912 0.14149 -0.16873
H*7 H 0.83222 0.24859 -0.03355
N8 N 0.84761 -0.23390 -0.31593
H*9 H 0.79612 -0.37788 -0.36727
H*10 H 0.93827 -0.22035 -0.36148
N'1+ N 0.22307 -0.25656 0.50300
N'2+ N 0.12487 0.08583 0.70925
N'3+ N 0.11164 -0.15137 0.60261
N4+ N 0.31199 -0.08380 0.54530
C5+ C 0.25181 0.12702 0.67217
C6+ C 0.32600 0.34201 0.74108
N'7+ N 0.45661 0.33314 0.67861
N'8+ N 0.49270 0.55764 0.76903
N'9+ N 0.38794 0.69424 0.88058
N'10+ N 0.28078 0.56267 0.86595
H*11+ H 0.40864 -0.11233 0.48865

#END

S9. Optimized crystal structure coordinates for 5 polymorphs of **1e** (ionic form).

data_AGH_BTO_0H_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 3.890
_cell_length_b 27.525
_cell_length_c 9.604
_cell_angle_alpha 90.00
_cell_angle_beta 58.81

```
_cell_angle_gamma              90.00
_cell_volume                  879.683
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.34142 0.60519 0.22574
N2 N 0.35619 0.64441 0.30511
H*3 H 0.34456 0.64138 0.41232
H*4 H 0.37942 0.67817 0.25979
N5 N 0.31043 0.56083 0.29031
H*6 H 0.29861 0.55753 0.39795
N7 N 0.35674 0.60922 0.08466
H*8 H 0.37998 0.64185 0.03245
H*9 H 0.34443 0.57837 0.02968
N10 N 0.29513 0.51999 0.20684
H*11 H 0.53227 0.49764 0.17689
H*12 H 0.03150 0.50184 0.27625
N'1+ N 0.58836 0.25648 -0.27174
N'2+ N 0.62531 0.19200 -0.41447
N'3+ N 0.59862 0.24131 -0.40181
N4+ N 0.60886 0.21604 -0.19688
C5+ C 0.63161 0.17632 -0.28445
C6+ C 0.65663 0.12808 -0.22996
N'7+ N 0.65739 0.12244 -0.09040
N'8+ N 0.68297 0.07443 -0.07739
N'9+ N 0.69682 0.05245 -0.20392
N'10+ N 0.68068 0.08550 -0.30278
H*11+ H 0.60697 0.21637 -0.09113

#END

data_AGH_BTO_0H_2
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 11.322
_cell_length_b                 4.194
_cell_length_c                 13.906
_cell_angle_alpha               132.62
_cell_angle_beta                92.19
_cell_angle_gamma              105.17
_cell_volume                   446.88
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.30844 0.67340 0.67886
N2 N 0.37310 0.40322 0.60439
H*3 H 0.45742 0.45269 0.64938
H*4 H 0.33919 0.14201 0.50096
N5 N 0.35694 1.01798 0.81654
H*6 H 0.44159 1.06951 0.86237
N7 N 0.19748 0.60801 0.61955
H*8 H 0.15808 0.35337 0.51665
H*9 H 0.15249 0.82243 0.68071
N10 N 0.28896 1.29906 0.89378
H*11 H 0.26400 1.26563 0.95700
H*12 H 0.34285 1.64218 0.94952
N'1+ N -0.01629 0.78236 0.15069
N'2+ N 0.09536 0.99227 0.33099
N'3+ N -0.00424 1.00590 0.27754
N4+ N 0.07797 0.61729 0.11990
C5+ C 0.14680 0.74597 0.23067
C6+ C 0.25410 0.61190 0.22442
N'7+ N 0.28629 0.35581 0.10712
N'8+ N 0.38701 0.29680 0.13699
N'9+ N 0.41360 0.50891 0.26660
N'10+ N 0.33101 0.71182 0.32473
H*11+ H 0.09289 0.42665 0.02708

#END

data_AGH_BTO_0H_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                 9.051
_cell_length_b                 3.685
_cell_length_c                 26.189
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   873.48
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.30765 -0.79391 -0.17311
N2 N 0.18468 -0.89765 -0.19756
H*3 H 0.10426 -1.03793 -0.17950
H*4 H 0.16900 -0.83824 -0.23482
N5 N 0.32430 -0.87852 -0.12343
H*6 H 0.24393 -1.01938 -0.10506
N7 N 0.41342 -0.60930 -0.19691
H*8 H 0.40493 -0.54088 -0.23413
H*9 H 0.50424 -0.53744 -0.17661
N10 N 0.45299 -0.76942 -0.09809
H*11 H 0.42742 -0.60056 -0.06859
H*12 H 0.50921 -0.99004 -0.08500
N'1+ N 0.02402 -0.73571 0.48974
N'2+ N -0.09406 -0.69608 0.56301
N'3+ N -0.10431 -0.69593 0.51113
N4+ N 0.12128 -0.76274 0.52862
C5+ C 0.04890 -0.73843 0.57374
C6+ C 0.12864 -0.75968 0.62161
N'7+ N 0.27677 -0.80421 0.62148
N'8+ N 0.31316 -0.81235 0.67090
N'9+ N 0.19176 -0.77426 0.69923
N'10+ N 0.07300 -0.74028 0.66908
H*11+ H 0.23134 -0.79609 0.52373

#END

data_AGH_BTO_0H_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                 3.930
_cell_length_b                 27.785
_cell_length_c                 9.577
_cell_angle_alpha               90.00
_cell_angle_beta                57.64
_cell_angle_gamma                90.00
_cell_volume                   883.356
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

C1 C -0.19896 0.35665 0.59590
N2 N -0.18812 0.39513 0.50929
H*3 H -0.17625 0.39153 0.40177
H*4 H -0.19153 0.42887 0.54924
N5 N -0.19393 0.31227 0.53835
H*6 H -0.18202 0.30841 0.43044
N7 N -0.21458 0.36142 0.73737
H*8 H -0.21882 0.39409 0.78446
H*9 H -0.22228 0.33111 0.79800
N10 N -0.20531 0.27221 0.62936
H*11 H -0.45563 0.25212 0.66471
H*12 H 0.04743 0.25189 0.56111
N'1+ N 0.29728 -0.00636 0.53986
N'2+ N 0.30074 0.05701 0.40115
N'3+ N 0.29856 0.00810 0.41071
N4+ N 0.29867 0.03415 0.61731
C5+ C 0.30081 0.07319 0.53222
C6+ C 0.30263 0.12135 0.58978
N'7+ N 0.30221 0.12761 0.72975
N'8+ N 0.30422 0.17535 0.74580
N'9+ N 0.30577 0.19659 0.62062
N'10+ N 0.30482 0.16331 0.51963
H*11+ H 0.29816 0.03432 0.72308

#END

data_AGH_BTO_0H_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 17.452
_cell_length_b 4.156
_cell_length_c 14.809
_cell_angle_alpha 90.00
_cell_angle_beta 129.23
_cell_angle_gamma 90.00
_cell_volume 832.016
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.05574 0.66194 0.27869
N2 N 0.03643 0.61350 0.17661

H*3 H -0.01659 0.45797 0.11693
H*4 H 0.07447 0.73150 0.15649
N5 N 0.00334 0.49983 0.30215
H*6 H -0.05002 0.34325 0.24259
N7 N 0.12553 0.86668 0.35716
H*8 H 0.16635 0.99257 0.34271
H*9 H 0.13714 0.89432 0.43302
N10 N 0.02384 0.55143 0.40892
H*11 H -0.03707 0.63953 0.39557
H*12 H 0.04629 0.34271 0.45531
N'1+ N 0.16430 -0.06969 -0.02150
N'2+ N 0.12769 -0.10771 0.09566
N'3+ N 0.10608 -0.20333 -0.00616
N4+ N 0.22587 0.11893 0.07280
C5+ C 0.20349 0.09595 0.14502
C6+ C 0.25903 0.27595 0.25310
N'7+ N 0.33401 0.46914 0.28262
N'8+ N 0.36809 0.59500 0.38497
N'9+ N 0.31557 0.48140 0.41504
N'10+ N 0.24588 0.27855 0.33320
H*11+ H 0.28006 0.25487 0.08552

#END

S10. Optimized crystal structure coordinates for 5 polymorphs of **1f** (ionic form).

data_DAGH_BTO_0H_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 17.330
_cell_length_b 9.100
_cell_length_c 5.924
_cell_angle_alpha 90.00
_cell_angle_beta 84.43
_cell_angle_gamma 90.00
_cell_volume 929.821
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.83778 0.34123 0.53727
N2 N 0.78007 0.30212 0.69233
H*3 H 0.77040 0.36589 0.83314
N4 N 0.88002 0.46177 0.57381

H*5 H 0.92385 0.49226 0.45730
N6 N 0.85312 0.26177 0.34934
H*7 H 0.81985 0.17198 0.32896
H*8 H 0.89626 0.28877 0.22973
N9 N 0.86229 0.54268 0.77317
N10 N 0.73635 0.17668 0.65340
H*11 H 0.67967 0.20471 0.64807
H*12 H 0.90851 0.54411 0.86690
H*13 H 0.84686 0.64715 0.73550
H*14 H 0.74117 0.10191 0.77917
N'1+ N -0.15532 -0.13404 0.75123
N'2+ N -0.15664 0.03872 1.01169
N'3+ N -0.19240 -0.08211 0.93493
N4+ N -0.09351 -0.04491 0.70601
C5+ C -0.09419 0.06146 0.86601
C6+ C -0.03371 0.17186 0.85623
N'7+ N 0.02411 0.16920 0.68610
N'8+ N 0.06859 0.28389 0.72869
N'9+ N 0.03847 0.35189 0.91627
N'10+ N -0.02641 0.28345 1.00104
H*11+ H -0.05348 -0.05806 0.57144

#END

data_DAGH_BTO_0H_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 9.064
_cell_length_b 16.249
_cell_length_c 3.962
_cell_angle_alpha 124.91
_cell_angle_beta 95.98
_cell_angle_gamma 81.59
_cell_volume 473.226
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.79403 0.30120 1.00668
N2 N 0.93312 0.29824 0.91211
H*3 H 0.99486 0.22989 0.75523
N4 N 0.74242 0.21469 0.89159
H*5 H 0.63719 0.21619 0.96186
N6 N 0.70796 0.38869 1.21203

H*7 H 0.75142 0.45185 1.29235
H*8 H 0.60273 0.39307 1.28725
N9 N 0.83593 0.12413 0.67617
N10 N 0.98616 0.38843 1.03260
H*11 H 1.01377 0.38411 0.77984
H*12 H 0.85385 0.09250 0.83855
H*13 H 0.79023 0.07530 0.39376
H*14 H 1.07724 0.40127 1.22359
N'1+ N 0.33219 0.01423 0.12766
N'2+ N 0.16046 0.14447 0.36973
N'3+ N 0.19675 0.04779 0.25777
N4+ N 0.38641 0.09095 0.15484
C5+ C 0.28096 0.17117 0.30369
C6+ C 0.31135 0.26373 0.36251
N'7+ N 0.44610 0.27054 0.26840
N'8+ N 0.43572 0.36392 0.35820
N'9+ N 0.30048 0.41067 0.49976
N'10+ N 0.21905 0.34910 0.50612
H*11+ H 0.49073 0.08713 0.07398

#END

data_DAGH_BTO_0H_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 15.054
_cell_length_b 18.348
_cell_length_c 3.945
_cell_angle_alpha 90.00
_cell_angle_beta 64.48
_cell_angle_gamma 90.00
_cell_volume 983.34
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.78709 0.36097 -0.01906
N2 N 0.78010 0.29068 -0.09534
H*3 H 0.84284 0.26472 -0.27024
N4 N 0.87573 0.39390 -0.17510
H*5 H 0.88175 0.44714 -0.11896
N6 N 0.70729 0.39778 0.20835

H*7 H 0.64216 0.37081 0.31937
H*8 H 0.71048 0.45079 0.27056
N9 N 0.95803 0.35357 -0.41274
N10 N 0.68775 0.25674 0.06772
H*11 H 0.68953 0.21419 0.23046
H*12 H 0.98832 0.37591 -0.67448
H*13 H 1.00873 0.35160 -0.30629
H*14 H 0.66916 0.23844 -0.13687
N'1+ N 0.49773 -0.42319 0.20215
N'2+ N 0.61332 -0.34043 0.08121
N'3+ N 0.51843 -0.36020 0.29982
N4+ N 0.58130 -0.44543 -0.08859
C5+ C 0.65252 -0.39461 -0.16353
C6+ C 0.74986 -0.40543 -0.46484
N'7+ N 0.77022 -0.46677 -0.67420
N'8+ N 0.86432 -0.45895 -0.92019
N'9+ N 0.89847 -0.39562 -0.85962
N'10+ N 0.82764 -0.36045 -0.57276
H*11+ H 0.58779 -0.49322 -0.22529

#END

data_DAGH_BTO_0H_4
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 9.100
_cell_length_b 10.585
_cell_length_c 8.235
_cell_angle_alpha 108.43
_cell_angle_beta 120.81
_cell_angle_gamma 44.27
_cell_volume 473.861
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.14343 0.37055 0.69408
N2 N -0.05357 0.43817 0.68516
H*3 H -0.14932 0.56121 0.73590
N4 N 0.20568 0.46704 0.76887
H*5 H 0.35463 0.41692 0.77622
N6 N 0.27595 0.20984 0.62971
H*7 H 0.22233 0.14202 0.57463
H*8 H 0.42525 0.15571 0.63471

N9 N 0.06228 0.63542 0.83515
N10 N -0.11739 0.33723 0.60726
H*11 H -0.27502 0.40951 0.49193
H*12 H 0.15137 0.63369 0.97636
H*13 H 0.00249 0.73613 0.76183
H*14 H -0.12649 0.30731 0.70596
N'1+ N 0.43618 0.17370 0.10910
N'2+ N 0.61670 0.27141 0.26248
N'3+ N 0.41838 0.30671 0.19753
N4+ N 0.65208 0.04754 0.11611
C5+ C 0.76349 0.10733 0.21041
C6+ C 0.99929 -0.00347 0.23766
N'7+ N 1.11007 -0.16830 0.16859
N'8+ N 1.31900 -0.23157 0.21809
N'9+ N 1.33190 -0.10947 0.31262
N'10+ N 1.13192 0.03661 0.32733
H*11+ H 0.71678 -0.07272 0.05835

#END

data_DAGH_BTO_0H_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 15.143
_cell_length_b 19.001
_cell_length_c 3.990
_cell_angle_alpha 90.00
_cell_angle_beta 54.04
_cell_angle_gamma 90.00
_cell_volume 929.264
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.49273 0.79568 -0.13976
N2 N 0.44277 0.84757 -0.19569
H*3 H 0.37465 0.83513 -0.17658
N4 N 0.45121 0.73007 -0.06159
H*5 H 0.48849 0.69042 -0.01878
N6 N 0.58236 0.80891 -0.16128
H*7 H 0.61068 0.85904 -0.22076
H*8 H 0.62162 0.77078 -0.12037

N9 N 0.35691 0.71807 -0.04113
N10 N 0.48633 0.91569 -0.27687
H*11 H 0.43047 0.94922 -0.05133
H*12 H 0.37253 0.68295 -0.26260
H*13 H 0.29570 0.69993 0.24462
H*14 H 0.50712 0.93227 -0.55737
N'1+ N -0.18633 -0.09818 0.58098
N'2+ N -0.30522 -0.01196 0.89509
N'3+ N -0.28607 -0.07883 0.74451
N4+ N -0.13862 -0.04252 0.62527
C5+ C -0.21160 0.01059 0.81844
C6+ C -0.18058 0.07665 0.90361
N'7+ N -0.07788 0.08566 0.78984
N'8+ N -0.07768 0.15101 0.91292
N'9+ N -0.17613 0.17965 1.09234
N'10+ N -0.24315 0.13380 1.09115
H*11+ H -0.05989 -0.04194 0.52611

#END

S11. Optimized crystal structure coordinates for 5 polymorphs of **1g** (ionic form).

data_TAGH_BTO_0H_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 10.021
_cell_length_b 8.458
_cell_length_c 12.827
_cell_angle_alpha 90.00
_cell_angle_beta 90.44
_cell_angle_gamma 90.00
_cell_volume 1087.15
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.31669 0.48461 0.49787
N2 N 0.31591 0.43729 0.59762
H*3 H 0.31454 0.31902 0.61167
N4 N 0.31850 0.63927 0.47503
H*5 H 0.31922 0.71687 0.53555
N6 N 0.31568 0.37727 0.42097
H*7 H 0.31633 0.41794 0.34640
N8 N 0.31929 0.68567 0.37016

N9 N 0.31700 0.55182 0.67656
H*10 H 0.39981 0.53848 0.72224
H*11 H 0.23700 0.75216 0.35388
H*12 H 0.40312 0.74953 0.35514
H*13 H 0.23369 0.54111 0.72099
N14 N 0.31380 0.21634 0.44689
H*15 H 0.23021 0.16450 0.41687
H*16 H 0.39633 0.16187 0.41812
N'1+ N -0.08276 0.42889 0.18757
N'2+ N 0.03712 0.61127 0.10943
N'3+ N -0.08722 0.55970 0.13474
N4+ N 0.04809 0.39352 0.19724
C5+ C 0.12205 0.50555 0.14922
C6+ C 0.26634 0.49507 0.14833
N'7+ N 0.32831 0.37251 0.19577
N'8+ N 0.45797 0.39964 0.18016
N'9+ N 0.47247 0.53275 0.12573
N'10+ N 0.35278 0.59599 0.10438
H*11+ H 0.08305 0.29692 0.23512

#END

data_TAGH_BTO_0H_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 8.195
_cell_length_b 19.385
_cell_length_c 6.441
_cell_angle_alpha 90.00
_cell_angle_beta 84.46
_cell_angle_gamma 90.00
_cell_volume 1018.44
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.07525 0.18045 0.08088
N2 N -0.18739 0.13710 0.17293
H*3 H -0.25798 0.15443 0.30074
N4 N 0.02103 0.16017 -0.08819
H*5 H 0.00518 0.11154 -0.14173
N6 N -0.05940 0.24409 0.15790

H*7 H 0.02703 0.27539 0.08362
N8 N 0.13729 0.20646 -0.18154
N9 N -0.20154 0.07086 0.08941
H*10 H -0.31640 0.06395 0.04516
H*11 H 0.25204 0.18649 -0.17920
H*12 H 0.11443 0.21576 -0.33161
H*13 H -0.17879 0.03468 0.19758
N14 N -0.16151 0.26404 0.33476
H*15 H -0.09260 0.27628 0.45288
H*16 H -0.23021 0.30555 0.30047
N'1+ N -0.29694 0.40014 0.32377
N'2+ N -0.29932 0.48407 0.55423
N'3+ N -0.35517 0.42022 0.50844
N4+ N -0.20018 0.45221 0.24605
C5+ C -0.20144 0.50391 0.38754
C6+ C -0.10682 0.56614 0.34191
N'7+ N -0.01614 0.57296 0.15649
N'8+ N 0.05338 0.63504 0.16682
N'9+ N 0.00603 0.66392 0.35066
N'10+ N -0.09557 0.62150 0.46512
H*11+ H -0.13739 0.45142 0.10288

#END

data_TAGH_BTO_0H_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 12.814
_cell_length_b 8.633
_cell_length_c 9.915
_cell_angle_alpha 90.00
_cell_angle_beta 88.55
_cell_angle_gamma 90.00
_cell_volume 1096.48
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.49966 0.00798 -0.17910
N2 N 0.42113 0.11062 -0.17793
H*3 H 0.34707 0.06835 -0.17668
N4 N 0.59883 0.05757 -0.18077

H*5 H 0.61119 0.17388 -0.18110
N6 N 0.47902 -0.14426 -0.17860
H*7 H 0.54072 -0.21830 -0.17953
N8 N 0.67950 -0.05204 -0.18197
N9 N 0.44477 0.26910 -0.17849
H*10 H 0.41376 0.32032 -0.09409
H*11 H 0.72524 -0.03891 -0.26668
H*12 H 0.72360 -0.03868 -0.09875
H*13 H 0.41540 0.32009 -0.26202
N14 N 0.37471 -0.19312 -0.17685
H*15 H 0.36080 -0.25759 -0.26051
H*16 H 0.35915 -0.25736 -0.09258
N'1+ N 0.11949 -0.05138 0.40692
N'2+ N 0.18286 0.14336 0.52246
N'3+ N 0.16187 0.08493 0.39849
N4+ N 0.11243 -0.08343 0.54007
C5+ C 0.15137 0.03620 0.61136
C6+ C 0.15287 0.03063 0.75734
N'7+ N 0.11512 -0.09495 0.82358
N'8+ N 0.12835 -0.06183 0.95365
N'9+ N 0.17213 0.07760 0.96429
N'10+ N 0.18862 0.13913 0.84157
H*11+ H 0.08221 -0.18293 0.57826

#END

data_TAGH_BTO_0H_4
_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 13.163
_cell_length_b 8.993
_cell_length_c 9.259
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1096.03
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74119 -0.28253 0.40000
N2 N 0.64548 -0.33127 0.38556

H*3 H 0.63293 -0.44217 0.39705
N4 N 0.76190 -0.13730 0.38588
H*5 H 0.70295 -0.06778 0.36423
N6 N 0.81618 -0.37901 0.42856
H*7 H 0.88769 -0.33762 0.43872
N8 N 0.86256 -0.08917 0.40147
N9 N 0.56846 -0.22818 0.35571
H*10 H 0.51573 -0.22953 0.43619
H*11 H 0.88652 -0.03965 0.30860
H*12 H 0.86768 -0.01572 0.48487
H*13 H 0.53458 -0.25345 0.25993
N14 N 0.79254 -0.53022 0.44282
H*15 H 0.83074 -0.59036 0.36708
H*16 H 0.81189 -0.56643 0.54334
N'1+ N 0.05590 0.78941 0.10506
N'2+ N 0.13392 0.89815 0.28689
N'3+ N 0.11030 0.90299 0.14377
N4+ N 0.04343 0.70768 0.22602
C5+ C 0.09137 0.77435 0.33804
C6+ C 0.08950 0.70862 0.48088
N'7+ N 0.03953 0.57945 0.50320
N'8+ N 0.05307 0.55163 0.64362
N'9+ N 0.10875 0.65972 0.70233
N'10+ N 0.13302 0.76087 0.60188
H*11+ H 0.00381 0.61134 0.22953

#END

data_TAGH_BTO_0H_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 14.204
_cell_length_b 4.580
_cell_length_c 10.865
_cell_angle_alpha 75.16
_cell_angle_beta 98.52
_cell_angle_gamma 58.54
_cell_volume 547.707
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.18732 0.88064 0.70112
N2 N -0.24549 0.89384 0.78851

H*3 H -0.33382 1.02998 0.74934
N4 N -0.07073 0.70457 0.74745
H*5 H -0.02968 0.58468 0.84951
N6 N -0.24575 1.04350 0.56741
H*7 H -0.19846 1.02725 0.50452
N8 N -0.01198 0.69472 0.65403
N9 N -0.18239 0.72144 0.92777
H*10 H -0.19176 0.51875 0.97325
H*11 H 0.02843 0.82057 0.66526
H*12 H 0.04881 0.42574 0.66865
H*13 H -0.21215 0.91357 0.96986
N14 N -0.36759 1.22576 0.52157
H*15 H -0.40882 1.50001 0.46317
H*16 H -0.38844 1.10519 0.46656
N'1+ N 0.48542 -0.03040 0.14541
N'2+ N 0.58307 -0.02688 0.32172
N'3+ N 0.49721 -0.05891 0.26956
N4+ N 0.56571 0.02180 0.11513
C5+ C 0.62591 0.02407 0.22344
C6+ C 0.71766 0.07574 0.21716
N'7+ N 0.74382 0.12229 0.10230
N'8+ N 0.83036 0.16118 0.13138
N'9+ N 0.85463 0.13870 0.25821
N'10+ N 0.78464 0.08459 0.31523
H*11+ H 0.57740 0.05372 0.02425

#END

S12. Optimized crystal structure coordinates for 5 polymorphs of **2a** (ionic form).

data_NH4_BTO_1H_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 8.816
_cell_length_b 11.094
_cell_length_c 12.181
_cell_angle_alpha 90.00
_cell_angle_beta 143.07
_cell_angle_gamma 90.00
_cell_volume 715.815
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

N1 N 0.67699 -0.00966 0.41178
H*2 H 0.68936 -0.09461 0.38569
H*3 H 0.85027 0.01548 0.54233
H*4 H 0.62151 0.05031 0.32006
H*5 H 0.54682 -0.00982 0.39905
N'1+ N 0.68667 0.14440 0.23750
N2+ N 0.71683 0.31594 0.17211
N'3+ N 0.60835 0.25796 0.19549
N'4+ N 0.84111 0.12566 0.24261
C5+ C 0.86090 0.23275 0.20177
C6+ C 1.01434 0.24728 0.19428
N7+ N 1.14401 0.15156 0.22888
N'8+ N 1.27434 0.18570 0.21425
N'9+ N 1.22396 0.29920 0.17189
N'10+ N 1.06404 0.34121 0.15804
O11+ O 0.68267 0.42697 0.13048
H*12+ H 1.14680 0.06676 0.26097

#END

data_NH4_BTO_1H_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 7.890
_cell_length_b 8.963
_cell_length_c 10.579
_cell_angle_alpha 90.00
_cell_angle_beta 120.18
_cell_angle_gamma 90.00
_cell_volume 646.718
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.63259 0.23846 0.56733
H*2 H 0.61900 0.13060 0.53044
H*3 H 0.50488 0.27039 0.56334
H*4 H 0.74681 0.24484 0.67330
H*5 H 0.65967 0.30801 0.50224
N'1+ N 0.10030 0.52362 0.21427
N2+ N 0.27347 0.45579 0.11822
N'3+ N 0.20447 0.57569 0.15703

```
N'4+ N 0.09817 0.37539 0.21459
C5+ C 0.20638 0.33209 0.15457
C6+ C 0.23711 0.17747 0.13670
N7+ N 0.15608 0.07076 0.18085
N'8+ N 0.20379 -0.06542 0.15371
N'9+ N 0.31088 -0.04090 0.09469
N'10+ N 0.33547 0.10757 0.08196
O11+ O 0.37984 0.46485 0.05951
H*12+ H 0.07236 0.08682 0.22719

#END

data_NH4_BTO_1H_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21'
_symmetry_Int_Tables_number      4
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,-z
_cell_length_a                  5.211
_cell_length_b                  8.955
_cell_length_c                  7.045
_cell_angle_alpha                90.00
_cell_angle_beta                100.90
_cell_angle_gamma                90.00
_cell_volume                    322.82
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.50314 0.67361 0.13892
H*2 H 0.38528 0.65966 0.00563
H*3 H 0.65053 0.74741 0.12756
H*4 H 0.39420 0.71486 0.23448
H*5 H 0.58255 0.57251 0.18801
N'1+ N -0.30824 0.95470 0.58226
N2+ N 0.05600 0.88344 0.75888
N'3+ N -0.08252 1.00451 0.68153
N'4+ N -0.32332 0.80683 0.59128
C5+ C -0.09580 0.76139 0.70170
C6+ C -0.04131 0.60646 0.74376
N7+ N -0.22161 0.50166 0.67150
N'8+ N -0.12963 0.36478 0.72897
N'9+ N 0.10035 0.38704 0.83321
N'10+ N 0.16334 0.53469 0.84643
O11+ O 0.28334 0.89029 0.86356
H*12+ H -0.39888 0.51941 0.58737
```

```
#END

data_NH4_BTO_1H_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                 10.528
_cell_length_b                 12.902
_cell_length_c                 7.191
_cell_angle_alpha               90.00
_cell_angle_beta                41.79
_cell_angle_gamma               90.00
_cell_volume                   650.922
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.33407 0.11857 0.54157
H*2 H -0.42244 0.13777 0.52936
H*3 H -0.22310 0.17047 0.42674
H*4 H -0.40956 0.12092 0.74639
H*5 H -0.28118 0.04512 0.46379
N'1+ N -0.28231 0.36473 0.38540
N2+ N -0.09583 0.48006 0.30144
N'3+ N -0.25906 0.46611 0.38117
N'4+ N -0.14188 0.31195 0.31215
C5+ C -0.02449 0.38370 0.25924
C6+ C 0.14513 0.35503 0.17329
N7+ N 0.19042 0.25335 0.14359
N'8+ N 0.35429 0.24464 0.06191
N'9+ N 0.40597 0.33887 0.04311
N'10+ N 0.28108 0.40973 0.10997
O11+ O -0.02985 0.56839 0.27514
H*12+ H 0.11629 0.19183 0.17584

#END

data_NH4_BTO_1H_5
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
```

```
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 11.870
_cell_length_b                 8.974
_cell_length_c                 8.180
_cell_angle_alpha               103.35
_cell_angle_beta                155.68
_cell_angle_gamma                86.77
_cell_volume                   322.312
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.67346 0.68491 0.16885
H*2 H -0.83098 0.58006 -0.11603
H*3 H -0.51437 0.65436 0.42894
H*4 H -0.57666 0.76973 0.22739
H*5 H -0.77184 0.73549 0.13510
N'1+ N 0.47085 0.37829 1.25635
N2+ N 0.64786 0.37468 1.24824
N'3+ N 0.67318 0.46955 1.44091
N'4+ N 0.31483 0.22837 0.95240
C5+ C 0.42449 0.22520 0.94548
C6+ C 0.30874 0.08111 0.65320
N7+ N 0.08301 -0.05648 0.37459
N'8+ N 0.01051 -0.17568 0.13270
N'9+ N 0.18858 -0.11104 0.26327
N'10+ N 0.37690 0.04751 0.58461
O11+ O 0.80894 0.42349 1.34673
H*12+ H -0.01982 -0.07156 0.34439

#END
```

S13. Optimized crystal structure coordinates for 5 polymorphs of 2**b** (ionic form).

```
data_NH3OH_BTO_1H_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                 9.973
_cell_length_b                 12.958
_cell_length_c                 9.544
_cell_angle_alpha               22.44
_cell_angle_beta                89.25
_cell_angle_gamma              105.22
_cell_volume                   326.933
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.33425 -0.07093 0.23933
H*2 H -0.37727 -0.28507 0.44151
H*3 H -0.19859 0.19151 -0.12127
H*4 H -0.43309 -0.05825 0.21957
O5 O -0.33210 -0.18972 0.52142
H*6 H -0.29180 0.00663 0.34163
N'1+ N -0.25863 -0.40999 1.30145
N2+ N -0.06903 0.14410 0.71024
N'3+ N -0.23393 -0.24168 1.20948
N'4+ N -0.11757 -0.15197 0.88554
C5+ C 0.00178 0.19585 0.51355
C6+ C 0.17259 0.54751 0.00384
N7+ N 0.21705 0.53418 -0.11254
N'8+ N 0.38231 0.89556 -0.60896
N'9+ N 0.43562 1.12013 -0.78587
N'10+ N 0.31045 0.91794 -0.42100
O11+ O -0.00137 0.39432 0.49111
H*12+ H 0.14149 0.29604 0.12577

#END

data_NH3OH_BTO_1H_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z
_cell_length_a                 14.098
_cell_length_b                 8.739
_cell_length_c                 10.851
_cell_angle_alpha               90.00
_cell_angle_beta                98.01
_cell_angle_gamma                 90.00
_cell_volume                   1323.83
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.17184 0.00435 0.53359
H*2 H -0.14391 -0.00884 0.62593
H*3 H -0.18832 0.11835 0.51707
H*4 H -0.12175 -0.03229 0.47911
O5 O -0.25425 -0.08811 0.51770
H*6 H -0.28309 -0.07883 0.43082
N'1+ N 0.57557 0.31698 0.12531
N2+ N 0.64641 0.20312 0.28949
N'3+ N 0.62445 0.34208 0.23707
N'4+ N 0.56465 0.16817 0.10244
C5+ C 0.60885 0.09611 0.20489
C6+ C 0.61181 -0.06778 0.21407
N7+ N 0.56932 -0.15401 0.11787
N'8+ N 0.58092 -0.30377 0.14665
N'9+ N 0.62921 -0.30720 0.25749
N'10+ N 0.64993 -0.16406 0.30293
O11+ O 0.69335 0.18430 0.39743
H*12+ H 0.53395 -0.11582 0.03616

#END

data_NH3OH_BTO_1H_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a                 9.726
_cell_length_b                 8.927
_cell_length_c                 7.912
_cell_angle_alpha               90.00
_cell_angle_beta                91.93
_cell_angle_gamma                 90.00
_cell_volume                   686.562
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.17510 -0.35303 -0.17876
H*2 H 0.14332 -0.24304 -0.17339
H*3 H 0.09272 -0.41873 -0.21833
H*4 H 0.25428 -0.36098 -0.26210
```

O5 O 0.21951 -0.38736 -0.01231
H*6 H 0.25069 -0.49136 -0.01185
N'1+ N 0.14520 -1.04800 -0.10342
N2+ N 0.14184 -0.80635 -0.11660
N'3+ N 0.07901 -0.93305 -0.17465
N'4+ N 0.24824 -1.00215 -0.00166
C5+ C 0.24677 -0.85086 -0.00927
C6+ C 0.34469 -0.76128 0.08557
N7+ N 0.44193 -0.82902 0.18610
N'8+ N 0.52218 -0.72397 0.26255
N'9+ N 0.47418 -0.59630 0.20909
N'10+ N 0.36446 -0.61376 0.09946
O11+ O 0.10473 -0.67453 -0.15927
H*12+ H 0.45511 -0.94037 0.20388

#END

data_NH3OH_BTO_1H_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 7.843
_cell_length_b 16.496
_cell_length_c 5.816
_cell_angle_alpha 90.00
_cell_angle_beta 82.78
_cell_angle_gamma 90.00
_cell_volume 746.497
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.68046 0.84575 0.97373
H*2 H 0.69619 0.90415 1.03040
H*3 H 0.77047 0.80886 1.03657
H*4 H 0.55729 0.82667 1.03287
O5 O 0.70743 0.85126 0.73065
H*6 H 0.69361 0.79683 0.66963
N'1+ N -0.25534 0.00416 0.10545
N2+ N -0.29234 0.13348 0.14231
N'3+ N -0.33350 0.06710 0.02255
N'4+ N -0.16517 0.02641 0.27365
C5+ C -0.18774 0.10735 0.29770

C6+ C -0.10849 0.15310 0.46556
N7+ N -0.00784 0.11472 0.60496
N'8+ N 0.05268 0.16913 0.74804
N'9+ N -0.01021 0.23847 0.69562
N'10+ N -0.11063 0.23156 0.52198
O11+ O -0.34561 0.20480 0.10755
H*12+ H 0.02011 0.05488 0.60606

#END

data_NH3OH_BTO_1H_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 8.638
_cell_length_b 9.091
_cell_length_c 10.322
_cell_angle_alpha 90.00
_cell_angle_beta 62.58
_cell_angle_gamma 90.00
_cell_volume 719.503
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.24505 0.90797 0.79639
H*2 H -0.19848 1.00009 0.82525
H*3 H -0.36876 0.88500 0.87814
H*4 H -0.24740 0.92816 0.69883
O5 O -0.12588 0.79617 0.78244
H*6 H -0.16551 0.70632 0.75499
N'1+ N 0.59055 0.66757 0.15307
N2+ N 0.60082 0.90490 0.14291
N'3+ N 0.56922 0.78239 0.08351
N'4+ N 0.63457 0.70951 0.25501
C5+ C 0.64125 0.85808 0.24929
C6+ C 0.68530 0.94311 0.34488
N7+ N 0.72150 0.87371 0.44421
N'8+ N 0.75912 0.97445 0.52167
N'9+ N 0.74578 1.10122 0.46998
N'10+ N 0.70042 1.08735 0.36054
O11+ O 0.59210 1.03542 0.10201
H*12+ H 0.72149 0.76401 0.46055

#END

S14. Optimized crystal structure coordinates for 5 polymorphs of 2**c** (ionic form).

```
data_N2H5_BTO_1H_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a                 9.072
_cell_length_b                 8.986
_cell_length_c                 19.444
_cell_angle_alpha               90.00
_cell_angle_beta               153.01
_cell_angle_gamma                90.00
_cell_volume                   719.371
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.90606 0.40296 0.55652
H*2 H 0.93270 0.35062 0.61431
H*3 H 0.88114 0.51469 0.55638
N4 N 0.60722 0.35092 0.40124
H*5 H 0.58073 0.40463 0.34425
H*6 H 0.63258 0.23962 0.40251
H*7 H 1.11500 0.38710 0.61492
N'1+ N -0.39583 0.45901 -0.13873
N2+ N -0.31477 0.69611 -0.09889
N'3+ N -0.40968 0.58402 -0.18068
N'4+ N -0.29634 0.48437 -0.03342
C5+ C -0.24507 0.63269 -0.00788
C6+ C -0.13456 0.70181 0.10039
N7+ N -0.07916 0.61711 0.18001
N'8+ N 0.02238 0.70471 0.27438
N'9+ N 0.02770 0.83873 0.25184
N'10+ N -0.06737 0.84242 0.14528
O11+ O -0.29917 0.83212 -0.11042
H*12+ H -0.10708 0.50566 0.17263

#END

data_N2H5_BTO_1H_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                   9.277
_cell_length_b                   9.062
_cell_length_c                   8.363
_cell_angle_alpha                 90.00
_cell_angle_beta                 93.73
_cell_angle_gamma                   90.00
_cell_volume                     701.573
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.21086 0.15636 -0.43439
H*2 H 0.23847 0.26556 -0.44637
H*3 H 0.30139 0.10326 -0.38568
N4 N 0.17695 0.09663 -0.59300
H*5 H 0.15124 -0.01217 -0.58018
H*6 H 0.08797 0.15105 -0.64122
H*7 H 0.13029 0.14882 -0.35517
N'1+ N 0.10352 0.70802 -0.11200
N2+ N 0.12827 0.94503 -0.10939
N'3+ N 0.04939 0.83179 -0.17589
N'4+ N 0.21400 0.73530 -0.00698
C5+ C 0.23014 0.88357 -0.00471
C6+ C 0.34051 0.95450 0.09624
N7+ N 0.43182 0.87162 0.19260
N'8+ N 0.52595 0.96070 0.27612
N'9+ N 0.49186 1.09382 0.23088
N'10+ N 0.37787 1.09547 0.11983
O11+ O 0.10577 1.08034 -0.14355
H*12+ H 0.43228 0.76043 0.20313

#END

data_N2H5_BTO_1H_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 19.626
_cell_length_b 9.280
_cell_length_c 9.387
_cell_angle_alpha 90.00
_cell_angle_beta 24.21
_cell_angle_gamma 90.00
_cell_volume 701.096
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.44717 0.67680 0.91190
H*2 H 0.38131 0.68929 0.94440
H*3 H 0.50733 0.77284 0.81545
N4 N 0.57170 0.56655 0.65170
H*5 H 0.63773 0.55596 0.61816
H*6 H 0.51099 0.47193 0.74784
H*7 H 0.36452 0.65849 1.15169
N'1+ N -0.13032 0.43940 0.39226
N2+ N -0.11751 0.67150 0.35479
N'3+ N -0.18952 0.55240 0.43499
N'4+ N -0.02309 0.47926 0.28797
C5+ C -0.01444 0.62454 0.26392
C6+ C 0.09055 0.70659 0.15707
N7+ N 0.18430 0.63765 0.07731
N'8+ N 0.27246 0.73526 -0.01558
N'9+ N 0.23250 0.85975 0.00796
N'10+ N 0.12042 0.84741 0.11374
O11+ O -0.14619 0.79953 0.36743
H*12+ H 0.19016 0.53024 0.08366

#END

data_N2H5_BTO_1H_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 21.845
_cell_length_b 9.022
_cell_length_c 10.994
_cell_angle_alpha 90.00

```
_cell_angle_beta                19.31
_cell_angle_gamma               90.00
_cell_volume                    716.502
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.48037 -0.38350 0.67550
H*2 H 0.38271 -0.32509 0.81028
H*3 H 0.44318 -0.49338 0.74013
N4 N 0.46916 -0.33797 0.82261
H*5 H 0.56507 -0.39764 0.69035
H*6 H 0.50425 -0.22839 0.76090
H*7 H 0.60751 -0.37006 0.39555
N'1+ N -0.10019 0.19060 0.80817
N2+ N -0.11363 0.42797 0.85724
N'3+ N -0.17355 0.31331 0.89991
N'4+ N 0.00474 0.21990 0.70770
C5+ C -0.00301 0.36842 0.73776
C6+ C 0.09482 0.44136 0.65095
N7+ N 0.19842 0.36021 0.53523
N'8+ N 0.27730 0.45100 0.47004
N'9+ N 0.22227 0.58343 0.54492
N'10+ N 0.10923 0.58297 0.65781
O11+ O -0.15754 0.56282 0.92137
H*12+ H 0.21667 0.24907 0.50030

#END

data_N2H5_BTO_1H_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                  7.808
_cell_length_b                  9.303
_cell_length_c                  9.782
_cell_angle_alpha               90.00
_cell_angle_beta                97.93
_cell_angle_gamma               90.00
_cell_volume                    703.749
loop_
_atom_site_label
_atom_site_type_symbol
```

_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.00466 0.33693 -0.34674
H*2 H -0.11188 0.32285 -0.41932
H*3 H 0.00929 0.24419 -0.28902
N4 N -0.03966 0.45381 -0.25683
H*5 H 0.06660 0.46603 -0.18417
H*6 H -0.05526 0.54514 -0.31522
H*7 H 0.10246 0.34908 -0.39692
N'1+ N -0.10879 -0.27036 0.61804
N2+ N -0.12777 -0.03889 0.62410
N'3+ N -0.18782 -0.15833 0.55328
N'4+ N -0.00003 -0.22954 0.72775
C5+ C -0.01123 -0.08464 0.73221
C6+ C 0.08921 -0.00180 0.83830
N7+ N 0.19888 -0.06956 0.93743
N'8+ N 0.27919 0.02862 1.02564
N'9+ N 0.21906 0.15230 0.98043
N'10+ N 0.10126 0.13886 0.86485
O11+ O -0.17636 0.08843 0.59046
H*12+ H 0.22024 -0.17656 0.94682

#END

S15. Optimized crystal structure coordinates for 5 polymorphs of **2d** (ionic form).

data_GH_BTO_1H_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a 4.073
_cell_length_b 10.676
_cell_length_c 18.491
_cell_angle_alpha 90.00
_cell_angle_beta 89.46
_cell_angle_gamma 90.00
_cell_volume 804.015
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.44205 -0.93393 0.68520
N2 N -0.56344 -0.84915 0.73150
H*3 H -0.49865 -0.84896 0.78412

H*4 H -0.72351 -0.78280 0.71521
N5 N -0.23058 -1.02069 0.70826
H*6 H -0.13591 -1.08560 0.67419
H*7 H -0.15926 -1.02386 0.76043
N8 N -0.53213 -0.93195 0.61585
H*9 H -0.69159 -0.86722 0.59729
H*10 H -0.44338 -0.99513 0.57997
N'1+ N 0.72222 0.18799 -0.12935
N2+ N 1.01889 0.29800 -0.05689
N'3+ N 0.92000 0.28659 -0.12653
N'4+ N 0.68756 0.13460 -0.06482
C5+ C 0.87274 0.20301 -0.01914
C6+ C 0.89572 0.17275 0.05630
N7+ N 0.72808 0.07293 0.08316
N'8+ N 0.78536 0.06221 0.15469
N'9+ N 0.98266 0.15345 0.17033
N'10+ N 1.05769 0.22428 0.11123
O11+ O 1.21167 0.38328 -0.03464
H*12+ H 0.58118 0.01391 0.05547

#END

data_GH_BTO_1H_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 13.946
_cell_length_b 13.385
_cell_length_c 4.736
_cell_angle_alpha 90.00
_cell_angle_beta 109.38
_cell_angle_gamma 90.00
_cell_volume 833.964
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.67714 0.46682 0.62334
N2 N 0.72391 0.38973 0.54496
H*3 H 0.77197 0.40010 0.42807
H*4 H 0.71255 0.31886 0.60033
N5 N 0.69360 0.55984 0.54702
H*6 H 0.65905 0.61914 0.60397

H*7 H 0.74107 0.57354 0.43017
N8 N 0.61391 0.45089 0.77804
H*9 H 0.60040 0.38122 0.83798
H*10 H 0.57780 0.50806 0.83952
N'1+ N 0.37192 0.15993 1.26037
N2+ N 0.44837 0.28442 1.13734
N'3+ N 0.37743 0.25891 1.26351
N'4+ N 0.43596 0.11973 1.13807
C5+ C 0.48413 0.19729 1.06044
C6+ C 0.55985 0.18240 0.92017
N7+ N 0.58442 0.08823 0.86275
N'8+ N 0.65669 0.09205 0.73127
N'9+ N 0.67500 0.18628 0.71040
N'10+ N 0.61694 0.24497 0.82425
O11+ O 0.47322 0.37406 1.10391
H*12+ H 0.55475 0.02370 0.90833

#END

data_GH_BTO_1H_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 8.868
_cell_length_b 10.808
_cell_length_c 4.601
_cell_angle_alpha 104.26
_cell_angle_beta 90.39
_cell_angle_gamma 72.49
_cell_volume 406.511
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.82622 0.30014 -0.02829
N2 N 0.89057 0.17627 0.00656
H*3 H 0.86293 0.09707 -0.12310
H*4 H 0.96871 0.15824 0.16357
N5 N 0.72312 0.32106 -0.23793
H*6 H 0.67311 0.41384 -0.26803
H*7 H 0.69220 0.24470 -0.37238
N8 N 0.86498 0.40309 0.14650
H*9 H 0.94262 0.38951 0.30625
H*10 H 0.81775 0.49748 0.12394
N'1+ N 0.24617 -0.02103 0.48553

N2+ N 0.16464 0.19436 0.55611
N'3+ N 0.14547 0.07761 0.39303
N'4+ N 0.33007 0.02596 0.70127
C5+ C 0.27963 0.16084 0.74669
C6+ C 0.34446 0.24654 0.96641
N7+ N 0.45961 0.19185 1.13456
N'8+ N 0.50249 0.29031 1.32473
N'9+ N 0.41510 0.40137 1.27179
N'10+ N 0.31559 0.37932 1.05207
O11+ O 0.08634 0.30977 0.52574
H*12+ H 0.50832 0.09330 1.12475

#END

data_GH_BTO_1H_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 13.369
_cell_length_b 19.289
_cell_length_c 4.671
_cell_angle_alpha 90.00
_cell_angle_beta 44.44
_cell_angle_gamma 90.00
_cell_volume 843.368
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.01291 0.18160 0.57634
N2 N 0.03145 0.11324 0.56861
H*3 H 0.10286 0.09386 0.56387
H*4 H -0.02540 0.07898 0.56730
N5 N 0.08964 0.22576 0.57790
H*6 H 0.07731 0.27760 0.58370
H*7 H 0.16218 0.20858 0.57334
N8 N -0.08236 0.20580 0.58250
H*9 H -0.14144 0.17334 0.58145
H*10 H -0.09805 0.25724 0.58838
N'1+ N 0.35384 -0.12820 0.44558
N2+ N 0.22182 -0.05741 0.47375
N'3+ N 0.25555 -0.12530 0.44210
N'4+ N 0.38576 -0.06539 0.47802

C5+ C 0.30345 -0.02076 0.49582
C6+ C 0.30901 0.05272 0.53218
N7+ N 0.39893 0.07875 0.54945
N'8+ N 0.38644 0.14845 0.58305
N'9+ N 0.29129 0.16383 0.58585
N'10+ N 0.24040 0.10633 0.55508
O11+ O 0.13042 -0.03560 0.47990
H*12+ H 0.46615 0.05167 0.53951

#END

data_GH_BTO_1H_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 8.115
_cell_length_b 19.281
_cell_length_c 6.690
_cell_angle_alpha 90.00
_cell_angle_beta 126.02
_cell_angle_gamma 90.00
_cell_volume 846.626
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.43505 -0.18113 0.53277
N2 N -0.40315 -0.11267 0.54813
H*3 H -0.51753 -0.07861 0.49076
H*4 H -0.26374 -0.09301 0.61755
N5 N -0.62117 -0.20570 0.44007
H*6 H -0.64860 -0.25722 0.42680
H*7 H -0.73982 -0.17345 0.38059
N8 N -0.28082 -0.22502 0.61011
H*9 H -0.13901 -0.20756 0.68075
H*10 H -0.30159 -0.27692 0.60017
N'1+ N 0.18681 0.37028 0.34608
N2+ N -0.06282 0.44043 0.22612
N'3+ N -0.00991 0.37247 0.25101
N'4+ N 0.26460 0.43362 0.38431
C5+ C 0.10908 0.47784 0.30959
C6+ C 0.13626 0.55171 0.32347
N7+ N 0.32248 0.57851 0.41375

N'8+ N 0.31261 0.64844 0.40968
N'9+ N 0.12491 0.66320 0.31910
N'10+ N 0.01019 0.60506 0.26307
O11+ O -0.24159 0.46167 0.13992
H*12+ H 0.45155 0.55180 0.47586

#END

S16. Optimized crystal structure coordinates for 5 polymorphs of **2e** (ionic form).

data_AGH_BTO_1H_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 20.486
_cell_length_b 8.772
_cell_length_c 5.141
_cell_angle_alpha 90.00
_cell_angle_beta 79.36
_cell_angle_gamma 90.00
_cell_volume 907.97
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.82961 0.43914 0.77058
N2 N 0.89262 0.48810 0.73167
H*3 H 0.90777 0.56560 0.85326
H*4 H 0.92678 0.44874 0.57929
N5 N 0.78560 0.49445 0.97609
H*6 H 0.80049 0.57232 1.09895
N7 N 0.80973 0.33714 0.61046
H*8 H 0.84127 0.29307 0.45435
H*9 H 0.76148 0.30397 0.64886
N10 N 0.71985 0.44288 1.01572
H*11 H 0.70763 0.39075 1.19516
H*12 H 0.68845 0.53154 1.00353
N'1+ N 0.39298 0.38075 -0.02609
N2+ N 0.45763 0.22780 0.13681
N'3+ N 0.39475 0.28339 0.16999
N'4+ N 0.45176 0.39123 -0.18553
C5+ C 0.49252 0.29571 -0.08470
C6+ C 0.56097 0.27679 -0.20639
N7+ N 0.58605 0.35636 -0.42885
N'8+ N 0.65081 0.32100 -0.50806

N'9+ N 0.66423 0.22257 -0.33711
N'10+ N 0.61023 0.19173 -0.14699
O11+ O 0.47707 0.13092 0.29046
H*12+ H 0.56148 0.43127 -0.52527

#END

data_AGH_BTO_1H_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 19.752
_cell_length_b 8.195
_cell_length_c 5.821
_cell_angle_alpha 90.00
_cell_angle_beta 95.95
_cell_angle_gamma 90.00
_cell_volume 937.155
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.32988 0.58954 0.66894
N2 N 0.39682 0.57712 0.65203
H*3 H 0.41486 0.51344 0.52278
H*4 H 0.43117 0.63123 0.76836
N5 N 0.28577 0.51557 0.51029
H*6 H 0.30355 0.45143 0.38004
N7 N 0.30620 0.67337 0.83910
H*8 H 0.33768 0.73047 0.96124
H*9 H 0.25507 0.67889 0.84382
N10 N 0.21590 0.52898 0.52886
H*11 H 0.19220 0.58499 0.38635
H*12 H 0.19534 0.41656 0.54896
N'1+ N 0.31670 0.24409 0.97889
N2+ N 0.41073 0.33424 1.15637
N'3+ N 0.34201 0.33355 1.15749
N'4+ N 0.36572 0.18644 0.86140
C5+ C 0.42478 0.24242 0.97159
C6+ C 0.48946 0.20433 0.89279
N7+ N 0.49206 0.10963 0.70264
N'8+ N 0.55751 0.08989 0.66065
N'9+ N 0.59329 0.17086 0.82182

N'10+ N 0.55343 0.24364 0.96933
O11+ O 0.45142 0.40886 1.30463
H*12+ H 0.45223 0.05970 0.60391

#END

data_AGH_BTO_1H_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 10.280
_cell_length_b 27.420
_cell_length_c 4.055
_cell_angle_alpha 90.00
_cell_angle_beta 53.15
_cell_angle_gamma 90.00
_cell_volume 914.649
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.30249 -0.39354 0.13303
N2 N 0.23408 -0.35403 0.10093
H*3 H 0.13720 -0.35684 0.09627
H*4 H 0.27763 -0.32026 0.08047
N5 N 0.24074 -0.43792 0.15961
H*6 H 0.14344 -0.44100 0.15510
N7 N 0.42998 -0.38980 0.13914
H*8 H 0.47965 -0.35717 0.11989
H*9 H 0.47707 -0.42087 0.16392
N10 N 0.31271 -0.47906 0.19307
H*11 H 0.23088 -0.49688 0.46244
H*12 H 0.35573 -0.50179 -0.05080
N'1+ N 0.02429 0.41896 -0.16016
N2+ N 0.23898 0.41762 -0.18009
N'3+ N 0.13573 0.44728 -0.19067
N'4+ N 0.05008 0.37223 -0.13018
C5+ C 0.18440 0.37110 -0.14245
C6+ C 0.24969 0.32615 -0.11754
N7+ N 0.17562 0.28336 -0.08060
N'8+ N 0.25717 0.24614 -0.06265
N'9+ N 0.37726 0.26615 -0.08823
N'10+ N 0.37761 0.31555 -0.12260

```
O11+ O 0.36119 0.43270 -0.20245
H*12+ H 0.07502 0.27876 -0.06762

#END

data_AGH_BTO_1H_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                 25.024
_cell_length_b                 11.116
_cell_length_c                 4.200
_cell_angle_alpha               90.00
_cell_angle_beta                53.43
_cell_angle_gamma                90.00
_cell_volume                   938.297
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.65102 0.10785 0.89195
N2 N 0.60413 0.04129 0.91556
H*3 H 0.57244 0.07762 0.86799
H*4 H 0.59919 -0.04725 0.98176
N5 N 0.65597 0.22560 0.80294
H*6 H 0.62428 0.26263 0.75481
N7 N 0.69271 0.05996 0.95462
H*8 H 0.69055 -0.02794 1.02200
H*9 H 0.72727 0.11437 0.93304
N10 N 0.70504 0.29466 0.77869
H*11 H 0.73695 0.32937 0.50091
H*12 H 0.68373 0.36208 0.98306
N'1+ N -0.15008 0.01961 0.73791
N2+ N -0.15675 0.20640 0.89967
N'3+ N -0.18864 0.11627 0.85669
N'4+ N -0.09455 0.04252 0.70146
C5+ C -0.09838 0.15938 0.80233
C6+ C -0.04652 0.21664 0.79808
N7+ N 0.00810 0.15264 0.69037
N'8+ N 0.04996 0.22396 0.70778
N'9+ N 0.02111 0.32824 0.82318
N'10+ N -0.03864 0.32804 0.88271
O11+ O -0.17971 0.31256 1.01077
```

```
H*12+ H 0.01754 0.06517 0.60830

#END

data_AGH_BTO_1H_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                 3.817
_cell_length_b                 11.921
_cell_length_c                 20.426
_cell_angle_alpha               90.00
_cell_angle_beta                98.15
_cell_angle_gamma               90.00
_cell_volume                   920.046
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.01627 0.93741 0.64415
N2 N 0.11223 1.02775 0.67851
H*3 H 0.25888 1.02032 0.72353
H*4 H 0.06585 1.10594 0.66028
N5 N 0.05159 0.83462 0.67021
H*6 H 0.19871 0.82658 0.71541
N7 N -0.20923 0.94727 0.58491
H*8 H -0.26568 1.02290 0.56375
H*9 H -0.30003 0.87618 0.56101
N10 N -0.08335 0.74057 0.63409
H*11 H 0.11804 0.69019 0.62411
H*12 H -0.24970 0.69718 0.65966
N'1+ N 0.57631 -0.56295 0.35855
N2+ N 0.62582 -0.39635 0.31931
N'3+ N 0.48700 -0.49994 0.30525
N'4+ N 0.76685 -0.50529 0.40669
C5+ C 0.79895 -0.40083 0.38246
C6+ C 0.99059 -0.31415 0.42109
N7+ N 1.14496 -0.33666 0.48372
N'8+ N 1.30926 -0.24371 0.51048
N'9+ N 1.25464 -0.16730 0.46496
N'10+ N 1.05893 -0.20697 0.40883
O11+ O 0.59118 -0.31434 0.27898
H*12+ H 1.14247 -0.41050 0.50804
```

#END

S17. Optimized crystal structure coordinates for 5 polymorphs of **2f** (ionic form).

```
data_DAGH_BTO_1H_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                 16.338
_cell_length_b                 11.747
_cell_length_c                 4.272
_cell_angle_alpha               98.77
_cell_angle_beta                68.45
_cell_angle_gamma              138.91
_cell_volume                   490.719
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.37706 0.06157 0.17787
N2 N 0.24940 -0.08321 0.38818
H*3 H 0.20578 -0.06600 0.59581
N4 N 0.44148 0.22174 0.24922
H*5 H 0.53821 0.33218 0.09139
N6 N 0.43939 0.04706 -0.09829
H*7 H 0.38702 -0.07605 -0.14185
H*8 H 0.53555 0.15398 -0.26104
N9 N 0.37291 0.23207 0.54160
N10 N 0.18294 -0.24938 0.31267
H*11 H 0.09954 -0.31091 0.27694
H*12 H 0.42147 0.28880 0.70600
H*13 H 0.36562 0.30273 0.47338
H*14 H 0.15526 -0.32481 0.50902
N'1+ N 0.02059 0.37035 -0.13515
N2+ N 0.22823 0.55881 -0.19954
N'3+ N 0.14312 0.53676 -0.27195
N'4+ N 0.02184 0.28292 0.02302
C5+ C 0.15161 0.40015 -0.01625
C6+ C 0.19210 0.35217 0.12287
N7+ N 0.09846 0.18491 0.29918
N'8+ N 0.15866 0.16974 0.40550
N'9+ N 0.28538 0.32425 0.29550
N'10+ N 0.31083 0.44130 0.11942
O11+ O 0.35448 0.70355 -0.29265
H*12+ H -0.00150 0.08425 0.34797
```

```
#END

data_DAGH_BTO_1H_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                 20.835
_cell_length_b                 9.470
_cell_length_c                 5.208
_cell_angle_alpha               90.00
_cell_angle_beta               108.92
_cell_angle_gamma               90.00
_cell_volume                   972.059
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.16524 0.73598 0.68680
N2 N -0.21876 0.70422 0.76479
H*3 H -0.23032 0.77146 0.89555
N4 N -0.12945 0.85406 0.78353
H*5 H -0.08882 0.87899 0.72560
N6 N -0.14771 0.65170 0.51569
H*7 H -0.17609 0.56402 0.44813
H*8 H -0.10761 0.67313 0.45363
N9 N -0.14931 0.94019 0.96300
N10 N -0.25578 0.58130 0.66354
H*11 H -0.30475 0.60670 0.55810
H*12 H -0.11140 0.94677 1.14443
H*13 H -0.16179 1.03828 0.88224
H*14 H -0.25448 0.51540 0.81967
N'1+ N -0.03324 0.71507 0.38826
N2+ N 0.05758 0.83878 0.44894
N'3+ N 0.00050 0.82641 0.51931
N'4+ N -0.00083 0.65430 0.23577
C5+ C 0.05612 0.73123 0.27276
C6+ C 0.10431 0.69649 0.13838
N7+ N 0.09294 0.58356 -0.03096
N'8+ N 0.14439 0.57093 -0.13385
N'9+ N 0.18561 0.67386 -0.02865
N'10+ N 0.16295 0.75428 0.14092
O11+ O 0.10196 0.93493 0.53786
H*12+ H 0.05280 0.51711 -0.07733
```

```
#END

data_DAGH_BTO_1H_3
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21'
_symmetry_Int_Tables_number      4
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,-z
_cell_length_a                 12.003
_cell_length_b                 12.955
_cell_length_c                 3.769
_cell_angle_alpha               90.00
_cell_angle_beta               125.23
_cell_angle_gamma               90.00
_cell_volume                   478.731
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.07894 0.50397 -0.24694
N2 N -0.18862 0.45914 -0.30346
H*3 H -0.17604 0.38856 -0.16710
N4 N 0.04183 0.45435 -0.01498
H*5 H 0.12550 0.48769 0.02958
N6 N -0.08935 0.59647 -0.41825
H*7 H -0.18220 0.63093 -0.59026
H*8 H -0.00833 0.63200 -0.38065
N9 N 0.04906 0.35723 0.16036
N10 N -0.31392 0.51111 -0.54494
H*11 H -0.34801 0.52423 -0.35634
H*12 H 0.07926 0.30293 0.03705
H*13 H 0.11485 0.35920 0.49014
H*14 H -0.38351 0.46809 -0.80837
N'1+ N 0.26484 0.25533 -0.00063
N2+ N 0.43436 0.35666 0.42321
N'3+ N 0.29683 0.35267 0.12930
N'4+ N 0.37506 0.19569 0.19483
C5+ C 0.48167 0.25865 0.46088
C6+ C 0.61919 0.22077 0.72805
N7+ N 0.64417 0.11911 0.71609
N'8+ N 0.77939 0.10100 0.99101
N'9+ N 0.83415 0.18971 1.16364
N'10+ N 0.73910 0.26604 1.01101
O11+ O 0.50026 0.43878 0.61526
H*12+ H 0.57482 0.06357 0.53371
```

```
#END

data_DAGH_BTO_1H_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                 23.703
_cell_length_b                 6.731
_cell_length_c                 13.592
_cell_angle_alpha               90.00
_cell_angle_beta               118.04
_cell_angle_gamma                90.00
_cell_volume                   1913.99
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74403 0.15539 0.25671
N2 N 0.68854 0.13550 0.25928
H*3 H 0.69024 0.12293 0.33516
N4 N 0.79902 0.15788 0.35343
H*5 H 0.84130 0.17288 0.35231
N6 N 0.74472 0.17248 0.15962
H*7 H 0.70221 0.16984 0.08897
H*8 H 0.78586 0.18764 0.15528
N9 N 0.79651 0.13956 0.45392
N10 N 0.63152 0.13301 0.15845
H*11 H 0.60302 0.24786 0.15645
H*12 H 0.82063 0.01597 0.49577
H*13 H 0.81531 0.26260 0.50191
H*14 H 0.60832 0.00181 0.15033
N'1+ N 0.33583 -0.19832 0.08447
N2+ N 0.41213 -0.00733 0.09686
N'3+ N 0.35172 -0.00944 0.08393
N'4+ N 0.38305 -0.31942 0.09715
C5+ C 0.43102 -0.20081 0.10497
C6+ C 0.49063 -0.28051 0.11944
N7+ N 0.49966 -0.48018 0.12556
N'8+ N 0.55864 -0.52117 0.13909
```

N'9+ N 0.58434 -0.35010 0.14103
N'10+ N 0.54410 -0.19702 0.12918
O11+ O 0.44260 0.15040 0.10011
H*12+ H 0.46817 -0.58584 0.12101

#END

data_DAGH_BTO_1H_5
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P c a 21'
_symmetry_Int_Tables_number 29
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,y,1/2+z
3 1/2+x,-y,z
4 -x,-y,1/2+z
_cell_length_a 19.647
_cell_length_b 3.771
_cell_length_c 13.122
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 972.194
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.03701 0.12710 0.37196
N2 N -0.09133 -0.01169 0.41892
H*3 H -0.08510 -0.10072 0.49144
N4 N 0.02279 0.14274 0.42210
H*5 H 0.06422 0.24743 0.38715
N6 N -0.04216 0.24803 0.27686
H*7 H -0.08814 0.23089 0.24211
H*8 H -0.00204 0.35390 0.23969
N9 N 0.02637 0.01320 0.52196
N10 N -0.15337 -0.02724 0.36640
H*11 H -0.18928 0.11569 0.40441
H*12 H 0.06040 -0.18988 0.52623
H*13 H 0.03987 0.21083 0.57081
H*14 H -0.16880 -0.28408 0.35994
N'1+ N 0.13197 0.54413 0.61734
N2+ N 0.21901 0.52183 0.51699
N'3+ N 0.15007 0.54698 0.51993
N'4+ N 0.18588 0.51830 0.67803
C5+ C 0.24060 0.50421 0.61569
C6+ C 0.30864 0.47528 0.65476
N7+ N 0.31898 0.46147 0.75695

N'8+ N 0.38629 0.43475 0.77617
N'9+ N 0.41560 0.43260 0.68759
N'10+ N 0.36964 0.45712 0.61027
O11+ O 0.25376 0.51701 0.43511
H*12+ H 0.28307 0.46932 0.81213

#END

S18. Optimized crystal structure coordinates for 5 polymorphs of **2g** (ionic form).

data_TAGH_BTO_1H_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 18.238
_cell_length_b 14.637
_cell_length_c 3.903
_cell_angle_alpha 90.00
_cell_angle_beta 74.85
_cell_angle_gamma 90.00
_cell_volume 1005.69
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.67244 0.48982 0.74854
N2 N 0.73891 0.47411 0.51045
H*3 H 0.76958 0.52923 0.39568
N4 N 0.62976 0.41954 0.90774
H*5 H 0.64980 0.35540 0.84066
N6 N 0.64864 0.57581 0.82743
H*7 H 0.59794 0.58483 1.00928
N8 N 0.56051 0.43777 1.15563
N9 N 0.76251 0.38362 0.43263
H*10 H 0.81281 0.37278 0.49356
H*11 H 0.51700 0.40951 1.07336
H*12 H 0.56111 0.41163 1.39669
H*13 H 0.76870 0.37066 0.17023
N14 N 0.69430 0.64807 0.65737
H*15 H 0.66546 0.68611 0.51703
H*16 H 0.70957 0.68823 0.84037
N'1+ N 0.38641 0.14251 -0.24534
N2+ N 0.46016 0.25730 -0.23395
N'3+ N 0.39250 0.23232 -0.28991
N'4+ N 0.44693 0.10777 -0.16296

```
C5+ C 0.49339 0.17929 -0.15533
C6+ C 0.56523 0.16779 -0.07436
N7+ N 0.58777 0.08312 -0.00304
N'8+ N 0.65651 0.08847 0.06515
N'9+ N 0.67472 0.17432 0.03539
N'10+ N 0.62005 0.22597 -0.05052
O11+ O 0.48456 0.33915 -0.25503
H*12+ H 0.55901 0.02388 0.00071

#END

data_TAGH_BTO_1H_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                 3.932
_cell_length_b                 17.636
_cell_length_c                 14.911
_cell_angle_alpha               90.00
_cell_angle_beta                98.91
_cell_angle_gamma               90.00
_cell_volume                   1021.52
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.01920 0.17345 0.48395
N2 N -0.00136 0.15122 0.56892
H*3 H -0.11236 0.10015 0.57715
N4 N 0.16322 0.24032 0.46931
H*5 H 0.25371 0.27249 0.52443
N6 N -0.10425 0.12882 0.41362
H*7 H -0.08375 0.14772 0.35027
N8 N 0.18159 0.26226 0.37986
N9 N 0.12957 0.19890 0.64126
H*10 H 0.32054 0.17190 0.68328
H*11 H 0.04955 0.31151 0.36514
H*12 H 0.43197 0.26959 0.37178
H*13 H -0.06187 0.21383 0.67664
N14 N -0.25356 0.05920 0.43072
H*15 H -0.50370 0.05790 0.40011
H*16 H -0.12129 0.01597 0.40675
N'1+ N 0.32555 0.61551 -0.34922
```

```
N2+ N 0.21447 0.54526 -0.23869
N'3+ N 0.35973 0.61159 -0.25941
N'4+ N 0.16480 0.55484 -0.38801
C5+ C 0.09441 0.51057 -0.31918
C6+ C -0.08037 0.43925 -0.33537
N7+ N -0.17896 0.41497 -0.42186
N'8+ N -0.33733 0.34712 -0.42092
N'9+ N -0.33373 0.33111 -0.33586
N'10+ N -0.17757 0.38640 -0.28046
O11+ O 0.20141 0.52305 -0.15805
H*12+ H -0.14345 0.44203 -0.47950

#END

data_TAGH_BTO_1H_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                 11.922
_cell_length_b                 11.521
_cell_length_c                 4.252
_cell_angle_alpha               78.14
_cell_angle_beta                77.88
_cell_angle_gamma                77.70
_cell_volume                   549.941
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.31925 0.31936 -0.51661
N2 N 0.26861 0.43571 -0.56411
H*3 H 0.32154 0.49830 -0.62943
N4 N 0.25344 0.23318 -0.43019
H*5 H 0.16550 0.25976 -0.40317
N6 N 0.43570 0.28919 -0.55553
H*7 H 0.47071 0.20002 -0.51723
N8 N 0.30849 0.11223 -0.38200
N9 N 0.14673 0.46488 -0.52189
H*10 H 0.12165 0.51117 -0.73431
H*11 H 0.28253 0.07246 -0.14834
H*12 H 0.28818 0.06768 -0.54009
H*13 H 0.11600 0.51595 -0.34256
N14 N 0.50253 0.38096 -0.64594
H*15 H 0.55074 0.37684 -0.47131
H*16 H 0.55639 0.37206 -0.86306
```

N'1+ N -0.24727 0.04382 -0.25399
N2+ N -0.28320 0.23195 -0.20758
N'3+ N -0.32404 0.14496 -0.29977
N'4+ N -0.15830 0.06082 -0.13627
C5+ C -0.18022 0.17849 -0.10655
C6+ C -0.10191 0.23035 0.01483
N7+ N -0.00288 0.16025 0.10297
N'8+ N 0.05700 0.22730 0.20899
N'9+ N -0.00470 0.33503 0.18494
N'10+ N -0.10370 0.34127 0.06607
O11+ O -0.33540 0.34095 -0.21933
H*12+ H 0.02443 0.07146 0.09381

#END

data_TAGH_BTO_1H_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 18.170
_cell_length_b 14.465
_cell_length_c 4.024
_cell_angle_alpha 90.00
_cell_angle_beta 101.76
_cell_angle_gamma 90.00
_cell_volume 1035.42
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.33689 -0.02668 0.80329
N2 N 0.27651 -0.04727 0.56259
H*3 H 0.24126 0.00534 0.46874
N4 N 0.38519 -0.09349 0.93566
H*5 H 0.37404 -0.15885 0.84672
N6 N 0.34897 0.06071 0.91162
H*7 H 0.39538 0.07347 1.09441
N8 N 0.44787 -0.07018 1.18693
N9 N 0.26516 -0.13914 0.45372
H*10 H 0.26494 -0.14347 0.20093
H*11 H 0.44637 -0.10529 1.40482
H*12 H 0.49599 -0.08606 1.10663
H*13 H 0.21531 -0.16270 0.49912

N14 N 0.29765 0.12928 0.76922
H*15 H 0.27455 0.15910 0.95321
H*16 H 0.32417 0.17833 0.65503
N'1+ N -0.11161 0.15590 0.51197
N2+ N -0.04597 0.26193 0.33024
N'3+ N -0.11106 0.24513 0.43614
N'4+ N -0.04993 0.11375 0.46045
C5+ C -0.00853 0.17975 0.34658
C6+ C 0.06289 0.15949 0.26291
N7+ N 0.09022 0.07193 0.29804
N'8+ N 0.15755 0.06894 0.20561
N'9+ N 0.17028 0.15273 0.11719
N'10+ N 0.11332 0.21112 0.14839
O11+ O -0.02692 0.34097 0.23690
H*12+ H 0.06550 0.01609 0.37986

#END

data_TAGH_BTO_1H_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 23.594
_cell_length_b 4.239
_cell_length_c 22.493
_cell_angle_alpha 90.00
_cell_angle_beta 100.01
_cell_angle_gamma 90.00
_cell_volume 2215.39
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.34030 0.67703 -0.33936
N2 N 0.28285 0.66415 -0.35486
H*3 H 0.26601 0.65124 -0.39957
N4 N 0.36473 0.69428 -0.28101
H*5 H 0.33821 0.69703 -0.24991
N6 N 0.37332 0.67266 -0.38221

H*7 H 0.41668 0.68281 -0.36860
N8 N 0.42486 0.70748 -0.26599
N9 N 0.24930 0.66907 -0.30922
H*10 H 0.22542 0.46813 -0.31083
H*11 H 0.43707 0.91130 -0.24337
H*12 H 0.43974 0.51919 -0.23972
H*13 H 0.22276 0.86024 -0.31448
N14 N 0.34674 0.65454 -0.44287
H*15 H 0.35707 0.84771 -0.46570
H*16 H 0.35974 0.45561 -0.46205
N'1+ N 0.37581 0.14147 -0.52229
N2+ N 0.35714 0.29702 -0.61508
N'3+ N 0.33693 0.12374 -0.57246
N'4+ N 0.42041 0.31820 -0.53022
C5+ C 0.40902 0.41648 -0.58825
C6+ C 0.44815 0.61497 -0.61339
N7+ N 0.49810 0.70810 -0.57838
N'8+ N 0.52793 0.89176 -0.61109
N'9+ N 0.49660 0.90829 -0.66443
N'10+ N 0.44688 0.74091 -0.66800
O11+ O 0.33057 0.33178 -0.66899
H*12+ H 0.51210 0.65295 -0.53455

#END

S19. Optimized crystal structure coordinates for 5 polymorphs of **3a** (ionic form).

data_03477_-1.77027E+02
_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 9.336
_cell_length_b 18.757
_cell_length_c 4.725
_cell_angle_alpha 90.00
_cell_angle_beta 122.86
_cell_angle_gamma 90.00
_cell_volume 695.032
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.27252 0.59287 0.62289
H*2 H -0.35937 0.57572 0.67779
H*3 H -0.31805 0.63796 0.47625

H*4 H -0.15876 0.60426 0.84298
H*5 H -0.25390 0.55355 0.49453
N'1+ N 0.26969 0.02419 1.30245
N'2+ N 0.14153 0.12536 1.02975
N3+ N 0.13409 0.06850 1.19235
N'4+ N 0.36776 0.05323 1.20830
C5+ C 0.28913 0.11346 1.04622
C6+ C 0.34572 0.16401 0.89580
N'7+ N 0.48301 0.16513 0.87645
N'8+ N 0.47017 0.22568 0.70573
N'9+ N 0.33338 0.26142 0.62016
N10+ N 0.25365 0.22327 0.73807
O11+ O 0.01529 0.05686 1.23946
H*12+ H 0.14221 0.23836 0.70824

#END

data_03407_-1.76427E+02
_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 13.920
_cell_length_b 9.603
_cell_length_c 5.506
_cell_angle_alpha 90.00
_cell_angle_beta 65.18
_cell_angle_gamma 90.00
_cell_volume 668.023
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.13378 -0.50995 0.33440
H*2 H -0.07681 -0.44143 0.33290
H*3 H -0.10839 -0.55801 0.15116
H*4 H -0.14720 -0.58366 0.48045
H*5 H -0.20273 -0.45670 0.37309
N'1+ N 0.15324 -0.25059 0.35547
N'2+ N 0.06955 -0.12504 0.16010
N3+ N 0.08940 -0.25285 0.22437
N'4+ N 0.17534 -0.11738 0.37665
C5+ C 0.12471 -0.04431 0.25900
C6+ C 0.12415 0.10532 0.23052

N'7+ N 0.17067 0.20666 0.30783
N'8+ N 0.14242 0.32782 0.22749
N'9+ N 0.08155 0.30623 0.10604
N10+ N 0.06932 0.16662 0.10634
O11+ O 0.05336 -0.36354 0.17033
H*12+ H 0.02526 0.11883 0.02430

#END

data_03628_-1.76358E+02
_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 12.165
_cell_length_b 15.704
_cell_length_c 4.199
_cell_angle_alpha 90.00
_cell_angle_beta 57.50
_cell_angle_gamma 90.00
_cell_volume 676.546
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.24428 0.01716 0.71115
H*2 H -0.20340 0.05411 0.82313
H*3 H -0.29509 0.05531 0.63487
H*4 H -0.17194 -0.01445 0.47732
H*5 H -0.30669 -0.02633 0.90928
N'1+ N 0.11285 0.11392 -0.20597
N'2+ N -0.06697 0.18336 0.22953
N3+ N -0.01959 0.11688 -0.00646
N'4+ N 0.15233 0.18044 -0.09581
C5+ C 0.04370 0.22097 0.16372
C6+ C 0.03535 0.29733 0.36800
N'7+ N 0.12706 0.34602 0.35756
N'8+ N 0.06258 0.40964 0.61117
N'9+ N -0.06277 0.40255 0.77509
N10+ N -0.08146 0.33213 0.62496
O11+ O -0.08911 0.06275 -0.04189
H*12+ H -0.17066 0.31059 0.70010

#END

```
data_02788_-1.76213E+02
_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                 9.862
_cell_length_b                 6.834
_cell_length_c                 5.678
_cell_angle_alpha               79.95
_cell_angle_beta                77.36
_cell_angle_gamma                 62.70
_cell_volume                   330.599
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.39888 -0.30142 0.75284
H*2 H -0.44813 -0.18922 0.88155
H*3 H -0.33111 -0.45419 0.82987
H*4 H -0.48437 -0.31052 0.68581
H*5 H -0.33191 -0.25175 0.61413
N'1+ N -0.20104 -0.21136 1.35654
N'2+ N -0.16021 -0.20056 0.95145
N3+ N -0.26318 -0.18111 1.15403
N'4+ N -0.05350 -0.25158 1.28280
C5+ C -0.03155 -0.24440 1.04089
C6+ C 0.11032 -0.27775 0.87658
N'7+ N 0.25048 -0.32218 0.91585
N'8+ N 0.33923 -0.33623 0.69355
N'9+ N 0.26149 -0.30303 0.52158
N10+ N 0.11712 -0.26596 0.63394
O11+ O -0.40239 -0.13945 1.15853
H*12+ H 0.03023 -0.23470 0.54438

#END

data_10363_-1.76092E+02
_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 9.315
_cell_length_b 10.309
_cell_length_c 8.128
_cell_angle_alpha 90.00
_cell_angle_beta 69.77
_cell_angle_gamma 90.00
_cell_volume 732.37
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.28774 -0.46699 0.59798
H*2 H 0.29709 -0.54828 0.52175
H*3 H 0.34322 -0.39079 0.52038
H*4 H 0.17418 -0.44410 0.65828
H*5 H 0.33648 -0.48479 0.69152
N'1+ N 0.49339 0.14650 0.21679
N'2+ N 0.63810 0.32389 0.12551
N3+ N 0.51106 0.27485 0.24344
N'4+ N 0.61251 0.11145 0.07749
C5+ C 0.69732 0.21855 0.02511
C6+ C 0.83899 0.23027 -0.12164
N'7+ N 0.92040 0.14382 -0.23898
N'8+ N 1.04374 0.20927 -0.34717
N'9+ N 1.04222 0.33028 -0.30267
N10+ N 0.91398 0.34502 -0.16085
O11+ O 0.41758 0.33957 0.36595
H*12+ H 0.88247 0.43034 -0.09705

#END

S20. Optimized crystal structure coordinates for 5 polymorphs of **3b** (ionic form).

data_04806_-1.84014E+02
_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 9.160
_cell_length_b 21.254
_cell_length_c 3.978
_cell_angle_alpha 90.00
_cell_angle_beta 64.29
_cell_angle_gamma 90.00

```
_cell_volume                  697.793
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.22767 0.41798 -0.11281
H*2 H 0.27472 0.45852 -0.05636
H*3 H 0.12480 0.42929 -0.14505
H*4 H 0.31406 0.39788 -0.35328
O5 O 0.19184 0.37948 0.20059
H*6 H 0.14666 0.34031 0.15813
N'1+ N 0.29526 0.52744 0.18222
N'2+ N 0.18560 0.62160 0.40308
N3+ N 0.16562 0.56614 0.26943
N'4+ N 0.40229 0.55880 0.26179
C5+ C 0.33460 0.61478 0.39300
C6+ C 0.40370 0.66569 0.51780
N'7+ N 0.54495 0.67118 0.53689
N'8+ N 0.54492 0.72958 0.67673
N'9+ N 0.41218 0.75991 0.74377
N10+ N 0.32201 0.72029 0.64512
O11+ O 0.04107 0.55101 0.22798
H*12+ H 0.21083 0.73138 0.66700

#END

data_01831_-1.84000E+02
_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                4.500
_cell_length_b                18.233
_cell_length_c                4.101
_cell_angle_alpha              90.00
_cell_angle_beta               81.70
_cell_angle_gamma               90.00
_cell_volume                  332.957
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.34992 -0.22935 0.21650
H*2 H 0.40291 -0.28214 0.13910
```

H*3 H 0.17620 -0.23119 0.41073
H*4 H 0.53793 -0.20521 0.28795
O5 O 0.26326 -0.19448 -0.06070
H*6 H 0.21084 -0.14396 0.00254
N'1+ N -0.38972 0.64322 -0.08069
N'2+ N 0.02049 0.62194 -0.44756
N3+ N -0.18382 0.67161 -0.32319
N'4+ N -0.31646 0.57311 -0.04716
C5+ C -0.07147 0.56155 -0.26798
C6+ C 0.09364 0.49368 -0.32707
N'7+ N 0.05243 0.42761 -0.18833
N'8+ N 0.27686 0.38456 -0.34215
N'9+ N 0.45197 0.42048 -0.56597
N10+ N 0.33953 0.48928 -0.55947
O11+ O -0.18697 0.73745 -0.41846
H*12+ H 0.43120 0.52992 -0.70925

#END

data_____-1.82744E+02
_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 4.443
_cell_length_b 21.241
_cell_length_c 7.987
_cell_angle_alpha 90.00
_cell_angle_beta 112.06
_cell_angle_gamma 90.00
_cell_volume 698.581
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.00146 -0.09820 -0.26415
H*2 H -0.05016 -0.13357 -0.35904
H*3 H -0.14696 -0.05993 -0.32172
H*4 H -0.04734 -0.11470 -0.15441
O5 O 0.32939 -0.08447 -0.21852
H*6 H 0.38584 -0.05094 -0.12828
N'1+ N 0.21925 0.52596 -0.19287
N'2+ N 0.13466 0.61274 -0.36395
N3+ N 0.02062 0.55606 -0.34436

N'4+ N 0.46919 0.56430 -0.11205
C5+ C 0.41409 0.61573 -0.21615
C6+ C 0.61709 0.67110 -0.18541
N'7+ N 0.89822 0.68587 -0.05367
N'8+ N 0.97746 0.74417 -0.09453
N'9+ N 0.76149 0.76571 -0.24314
N10+ N 0.53299 0.72023 -0.30200
O11+ O -0.24122 0.53277 -0.45333
H*12+ H 0.33265 0.72399 -0.41646

#END

data_02557_-1.82718E+02
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P 1'
_symmetry_Int_Tables_number 1
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
_cell_length_a 15.725
_cell_length_b 5.584
_cell_length_c 3.929
_cell_angle_alpha 126.57
_cell_angle_beta 135.98
_cell_angle_gamma 44.52
_cell_volume 165.636
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.43219 0.13444 0.51672
H*2 H 0.53347 0.05866 0.66137
H*3 H 0.43797 -0.04497 0.55549
H*4 H 0.38829 0.37697 0.70552
O5 O 0.35870 0.14066 0.01441
H*6 H 0.26156 0.21174 -0.13745
N'1+ N 0.68258 0.00720 -0.20490
N'2+ N 0.73186 0.33949 -0.11271
N3+ N 0.62967 0.30946 -0.27704
N'4+ N 0.82316 -0.16338 0.01252
C5+ C 0.85031 0.03905 0.06410
C6+ C 0.98801 -0.03283 0.28095
N'7+ N 1.11861 -0.30272 0.47839
N'8+ N 1.20798 -0.22980 0.62400
N'9+ N 1.13959 0.06808 0.52698
N10+ N 1.00094 0.19533 0.31088
O11+ O 0.49878 0.53461 -0.47676
H*12+ H 0.92174 0.42698 0.19391

#END

data_01675_-1.82366E+02
_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 22.300
_cell_length_b 9.231
_cell_length_c 6.791
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1397.94
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.09011 -0.16667 -0.24510
H*2 H 0.06909 -0.25741 -0.30041
H*3 H 0.10596 -0.10534 -0.36121
H*4 H 0.05966 -0.10837 -0.16229
O5 O 0.13709 -0.22132 -0.12874
H*6 H 0.15830 -0.13827 -0.07317
N'1+ N 0.52999 0.31960 -0.15254
N'2+ N 0.62451 0.38316 -0.08151
N3+ N 0.56911 0.43032 -0.12172
N'4+ N 0.56099 0.19719 -0.13166
C5+ C 0.61720 0.23746 -0.08938
C6+ C 0.66787 0.14341 -0.05346
N'7+ N 0.67290 -0.00057 -0.05216
N'8+ N 0.73131 -0.02914 -0.00942
N'9+ N 0.76207 0.08877 0.01534
N10+ N 0.72276 0.19837 -0.01191
O11+ O 0.55440 0.56230 -0.13038
H*12+ H 0.73421 0.30414 -0.00165

#END

S21. Optimized crystal structure coordinates for 5 polymorphs of **3c** (ionic form).

data_07138_-1.78620E+02

```
_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                 10.179
_cell_length_b                 9.066
_cell_length_c                 8.017
_cell_angle_alpha               90.00
_cell_angle_beta                90.61
_cell_angle_gamma                 90.00
_cell_volume                   739.789
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.23480 0.84135 0.88767
H*2 H -0.26140 0.73606 0.92115
H*3 H -0.32042 0.89715 0.86071
N4 N -0.15873 0.83238 0.73641
H*5 H -0.13398 0.93743 0.70299
H*6 H -0.07463 0.77543 0.76379
H*7 H -0.18916 0.89143 0.98844
N'1+ N 0.08111 0.72145 -0.13199
N'2+ N 0.25263 0.80912 0.01472
N3+ N 0.14803 0.84321 -0.08012
N'4+ N 0.14427 0.60514 -0.06883
C5+ C 0.24615 0.65978 0.01815
C6+ C 0.34429 0.57704 0.11026
N'7+ N 0.36052 0.43249 0.13353
N'8+ N 0.46978 0.41796 0.23130
N'9+ N 0.52092 0.54494 0.26884
N10+ N 0.44301 0.64622 0.19354
O11+ O 0.11449 0.97323 -0.11785
H*12+ H 0.45907 0.75615 0.20102

#END

data_06460_-1.78334E+02
_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 8.233
_cell_length_b 8.967
_cell_length_c 9.669
_cell_angle_alpha 90.00
_cell_angle_beta 87.41
_cell_angle_gamma 90.00
_cell_volume 713.088
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.02644 0.59018 -0.30569
H*2 H -0.07500 0.63226 -0.21389
H*3 H 0.00001 0.47988 -0.28805
N4 N 0.12475 0.66757 -0.33868
H*5 H 0.17308 0.62401 -0.42909
H*6 H 0.09763 0.77726 -0.35451
H*7 H -0.11336 0.59600 -0.37924
N'1+ N 0.32937 0.59768 0.43027
N'2+ N 0.50706 0.69947 0.27532
N3+ N 0.40103 0.72509 0.38163
N'4+ N 0.39084 0.48634 0.35317
C5+ C 0.49645 0.54937 0.26148
C6+ C 0.59458 0.47450 0.15490
N'7+ N 0.60732 0.33105 0.11962
N'8+ N 0.71863 0.32540 0.01143
N'9+ N 0.77430 0.45674 -0.02116
N10+ N 0.69735 0.55183 0.06825
O11+ O 0.37021 0.85257 0.43178
H*12+ H 0.71670 0.66324 0.06747

#END

data_04542_-1.78005E+02
_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 21.610
_cell_length_b 9.007

```
_cell_length_c                  10.394
_cell_angle_alpha                 90.00
_cell_angle_beta                 20.96
_cell_angle_gamma                   90.00
_cell_volume                    723.696
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.46236 0.32411 0.88819
H*2 H 0.48542 0.21211 0.83452
H*3 H 0.41743 0.35995 0.88761
N4 N 0.62577 0.39723 0.59593
H*5 H 0.60205 0.50850 0.64924
H*6 H 0.67043 0.35981 0.59585
H*7 H 0.36661 0.33996 1.14200
N'1+ N -0.15818 0.32603 0.38462
N'2+ N -0.00769 0.42656 0.25478
N3+ N -0.10856 0.45309 0.34858
N'4+ N -0.08731 0.21397 0.31200
C5+ C 0.00180 0.27626 0.23531
C6+ C 0.10173 0.20045 0.13883
N'7+ N 0.13186 0.05662 0.10103
N'8+ N 0.23502 0.05005 0.00658
N'9+ N 0.26941 0.18119 -0.01530
N10+ N 0.18639 0.27709 0.06723
O11+ O -0.15329 0.58107 0.39853
H*12+ H 0.18990 0.38855 0.07206

#END

data_07174_-1.77631E+02
_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                  11.770
_cell_length_b                  9.041
_cell_length_c                  7.288
_cell_angle_alpha                 90.00
_cell_angle_beta                 83.32
_cell_angle_gamma                   90.00
_cell_volume                    770.27
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.92800 0.09354 0.70060
H*2 H 1.01135 0.12941 0.67657
H*3 H 0.93084 -0.01382 0.74657
N4 N 0.88040 0.09260 0.52611
H*5 H 0.79811 0.05530 0.55082
H*6 H 0.87907 0.19934 0.48042
H*7 H 0.88532 0.15742 0.80410
N'1+ N -0.14984 0.48497 0.39621
N'2+ N 0.01124 0.56861 0.23557
N3+ N -0.08801 0.60552 0.33338
N'4+ N -0.08879 0.36657 0.33731
C5+ C 0.00685 0.41882 0.24190
C6+ C 0.10056 0.33323 0.15022
N'7+ N 0.11758 0.18767 0.13528
N'8+ N 0.22099 0.17028 0.03308
N'9+ N 0.26784 0.29647 -0.01499
N10+ N 0.19304 0.40016 0.05773
O11+ O -0.12122 0.73693 0.36454
H*12+ H 0.20693 0.51013 0.04252

#END

data_02765_-1.77326E+02
_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                 4.185
_cell_length_b                 17.850
_cell_length_c                 5.770
_cell_angle_alpha               90.00
_cell_angle_beta                55.24
_cell_angle_gamma                 90.00
_cell_volume                   354.113
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.01175 -0.09631 0.29122
H*2 H -0.04001 -0.09922 0.13727
H*3 H 0.03012 -0.15063 0.34222
```

N4 N -0.32192 -0.06146 0.53797
H*5 H -0.27013 -0.05956 0.69080
H*6 H -0.34066 -0.00785 0.48468
H*7 H 0.27627 -0.07027 0.20847
N'1+ N 0.00621 0.77948 -0.41297
N'2+ N 0.02381 0.75885 -0.03737
N3+ N -0.06135 0.80788 -0.17006
N'4+ N 0.13901 0.71002 -0.43818
C5+ C 0.14728 0.69884 -0.21227
C6+ C 0.27032 0.63171 -0.14362
N'7+ N 0.40192 0.56613 -0.27629
N'8+ N 0.47295 0.52370 -0.11450
N'9+ N 0.39247 0.55952 0.10847
N10+ N 0.26453 0.62763 0.09315
O11+ O -0.18989 0.87318 -0.08155
H*12+ H 0.17970 0.66805 0.24026

#END

S22. Optimized crystal structure coordinates for 5 polymorphs of **3d** (ionic form).

data_06550_-1.68081E+02
_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 7.282
_cell_length_b 13.435
_cell_length_c 8.678
_cell_angle_alpha 90.00
_cell_angle_beta 97.99
_cell_angle_gamma 90.00
_cell_volume 840.759
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.35203 -0.15425 0.70556
N2 N -0.32114 -0.07279 0.62438
H*3 H -0.27189 -0.07767 0.52136
H*4 H -0.34615 -0.00399 0.66369
N5 N -0.31769 -0.24438 0.65071
H*6 H -0.34005 -0.30689 0.71017
H*7 H -0.26837 -0.25262 0.54821
N8 N -0.41726 -0.14557 0.84158
H*9 H -0.44415 -0.07819 0.88515

H*10 H -0.44157 -0.20614 0.90478
N'1+ N 0.34133 0.86593 0.31627
N'2+ N 0.42969 0.76680 0.13237
N3+ N 0.40839 0.86076 0.17784
N'4+ N 0.31857 0.77256 0.36171
C5+ C 0.37201 0.71466 0.25053
C6+ C 0.37310 0.60708 0.24652
N'7+ N 0.32459 0.53920 0.34552
N'8+ N 0.35468 0.44913 0.28198
N'9+ N 0.41855 0.45816 0.15036
N10+ N 0.43093 0.55719 0.12642
O11+ O 0.44588 0.93646 0.10172
H*12+ H 0.47705 0.58684 0.03174

#END

data_01613_-1.67683E+02
_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 16.153
_cell_length_b 11.855
_cell_length_c 4.910
_cell_angle_alpha 90.00
_cell_angle_beta 116.49
_cell_angle_gamma 90.00
_cell_volume 841.521
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.66300 0.55154 0.14281
N2 N 0.60463 0.56804 0.26469
H*3 H 0.58473 0.64646 0.29090
H*4 H 0.57873 0.50256 0.33415
N5 N 0.69621 0.63979 0.05287
H*6 H 0.74038 0.62921 -0.03978
H*7 H 0.67810 0.71962 0.07493
N8 N 0.68816 0.44680 0.11087
H*9 H 0.66389 0.37894 0.17731
H*10 H 0.73218 0.43244 0.01936
N'1+ N 0.31829 0.03682 0.86822
N'2+ N 0.41647 0.01666 0.66257

N3+ N 0.37247 0.08963 0.76061
N'4+ N 0.32750 -0.07358 0.83894
C5+ C 0.38629 -0.08377 0.71600
C6+ C 0.41837 -0.18741 0.63989
N'7+ N 0.39994 -0.29523 0.66822
N'8+ N 0.44972 -0.35684 0.55923
N'9+ N 0.49728 -0.29298 0.46640
N10+ N 0.47827 -0.18603 0.51568
O11+ O 0.37996 0.19555 0.75481
H*12+ H 0.50591 -0.11743 0.46463

#END

data_00952_-1.67650E+02
_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 7.110
_cell_length_b 13.424
_cell_length_c 17.778
_cell_angle_alpha 90.00
_cell_angle_beta 84.95
_cell_angle_gamma 90.00
_cell_volume 1690.23
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.14653 0.34463 -0.14741
N2 N -0.17087 0.25437 -0.17688
H*3 H -0.21857 0.24615 -0.22841
H*4 H -0.14228 0.19174 -0.14847
N5 N -0.18552 0.42625 -0.18628
H*6 H -0.16813 0.49515 -0.16507
H*7 H -0.23350 0.42140 -0.23800
N8 N -0.08320 0.35327 -0.07907
H*9 H -0.05289 0.29258 -0.04875
H*10 H -0.06381 0.42075 -0.05576
N'1+ N 0.16993 0.63307 0.65576

N'2+ N 0.07523 0.73235 0.56508
N3+ N 0.09998 0.63830 0.58710
N'4+ N 0.19107 0.72649 0.67886
C5+ C 0.13385 0.78447 0.62402
C6+ C 0.12977 0.89214 0.62265
N'7+ N 0.17842 0.96002 0.67217
N'8+ N 0.14463 1.05019 0.64116
N'9+ N 0.07838 1.04120 0.57579
N10+ N 0.06820 0.94211 0.56334
O11+ O 0.06302 0.56257 0.54889
H*12+ H 0.02099 0.91248 0.51618

#END

data_01913_-1.67383E+02
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 23.356
_cell_length_b 11.688
_cell_length_c 6.885
_cell_angle_alpha 90.00
_cell_angle_beta 152.37
_cell_angle_gamma 90.00
_cell_volume 871.637
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.33863 0.95733 1.01240
N2 N -0.32693 0.84867 0.98956
H*3 H -0.36141 0.78344 0.96560
H*4 H -0.28327 0.82860 0.99561
N5 N -0.39687 0.98138 1.00369
H*6 H -0.40674 1.06288 1.02055
H*7 H -0.43272 0.91876 0.98000
N8 N -0.29209 1.04194 1.04395
H*9 H -0.24775 1.02567 1.05106
H*10 H -0.29990 1.12463 1.06159
N'1+ N 0.48984 0.18585 0.03032
N'2+ N 0.51091 0.36763 -0.00424
N3+ N 0.46883 0.29795 0.00857
N'4+ N 0.54719 0.18290 0.03162

C5+ C 0.55885 0.29208 0.01085
C6+ C 0.61527 0.33359 0.00362
N'7+ N 0.66828 0.27890 0.01477
N'8+ N 0.70519 0.36159 -0.00060
N'9+ N 0.67782 0.46321 -0.02042
N10+ N 0.62115 0.44701 -0.01804
O11+ O 0.41559 0.33161 0.00144
H*12+ H 0.58916 0.51187 -0.03088

#END

data_04373_-1.67272E+02
_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 9.498
_cell_length_b 19.467
_cell_length_c 4.567
_cell_angle_alpha 90.00
_cell_angle_beta 96.18
_cell_angle_gamma 90.00
_cell_volume 839.52
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.32495 -0.08681 0.37219
N2 N 0.21145 -0.04724 0.39399
H*3 H 0.12326 -0.05182 0.25042
H*4 H 0.21057 -0.01160 0.55468
N5 N 0.32316 -0.13357 0.15727
H*6 H 0.40775 -0.16399 0.13680
H*7 H 0.23715 -0.13984 0.00906
N8 N 0.44024 -0.07962 0.56530
H*9 H 0.44384 -0.04461 0.72934
H*10 H 0.52714 -0.10899 0.55283
N'1+ N 0.34399 0.54785 0.17685
N'2+ N 0.25304 0.62696 -0.14622
N3+ N 0.22447 0.57697 0.03957
N'4+ N 0.45311 0.57996 0.07694
C5+ C 0.39662 0.62690 -0.11528
C6+ C 0.47214 0.67482 -0.28309
N'7+ N 0.61022 0.68537 -0.29406

N'8+ N 0.61983 0.73716 -0.49082
N'9+ N 0.49594 0.75873 -0.60007
N10+ N 0.40182 0.71998 -0.47143
O11+ O 0.10102 0.55855 0.08386
H*12+ H 0.29568 0.72534 -0.51472

#END

S23. Optimized crystal structure coordinates for 5 polymorphs of **3e** (ionic form).

data_____-1.71505E+02
_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 13.284
_cell_length_b 20.154
_cell_length_c 4.153
_cell_angle_alpha 90.00
_cell_angle_beta 124.51
_cell_angle_gamma 90.00
_cell_volume 916.207
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.59930 0.65844 0.20563
N2 N 0.51765 0.69681 0.20967
H*3 H 0.44770 0.67693 0.20898
H*4 H 0.52383 0.74679 0.21353
N5 N 0.58782 0.59201 0.20054
H*6 H 0.51776 0.57172 0.19982
N7 N 0.69132 0.68466 0.20655
H*8 H 0.70295 0.73423 0.21031
H*9 H 0.75054 0.65336 0.20335
N10 N 0.67339 0.55219 0.19634
H*11 H 0.71815 0.52276 0.43818
H*12 H 0.63125 0.52387 -0.05008
N'1+ N 0.18115 0.15523 -0.22275
N'2+ N 0.25709 0.06667 -0.34263
N3+ N 0.16958 0.08923 -0.30468
N'4+ N 0.27903 0.17599 -0.20724
C5+ C 0.32292 0.12247 -0.27947
C6+ C 0.42891 0.11953 -0.29470
N'7+ N 0.50800 0.16605 -0.24468
N'8+ N 0.58949 0.13492 -0.29278

N'9+ N 0.56468 0.07230 -0.36901
N10+ N 0.46380 0.06184 -0.37121
O11+ O 0.08550 0.05369 -0.34032
H*12+ H 0.42305 0.01701 -0.42327

#END

data_02665_-1.69562E+02
_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 4.193
_cell_length_b 10.340
_cell_length_c 20.757
_cell_angle_alpha 90.00
_cell_angle_beta 103.81
_cell_angle_gamma 90.00
_cell_volume 873.918
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.29388 0.40436 0.15911
N2 N -0.08377 0.48695 0.19709
H*3 H 0.03589 0.55487 0.17691
H*4 H -0.03919 0.48353 0.24708
N5 N -0.34648 0.41212 0.09265
H*6 H -0.22707 0.48013 0.07206
N7 N -0.45123 0.31501 0.18572
H*8 H -0.41821 0.30620 0.23533
H*9 H -0.60757 0.25493 0.15471
N10 N -0.56622 0.32560 0.05323
H*11 H -0.75573 0.37468 0.02339
H*12 H -0.44810 0.27083 0.02536
N'1+ N 0.27553 0.68874 0.15624
N'2+ N 0.43159 0.76282 0.06706
N3+ N 0.25101 0.67542 0.09006
N'4+ N 0.47795 0.78768 0.17667
C5+ C 0.56813 0.83044 0.12277
C6+ C 0.78707 0.93691 0.11939
N'7+ N 0.95093 1.01764 0.16574
N'8+ N 1.11898 1.09875 0.13416
N'9+ N 1.06714 1.07221 0.07142

N10+ N 0.85861 0.97051 0.06135
O11+ O 0.07694 0.58997 0.05474
H*12+ H 0.77399 0.92839 0.01653

#END

data_01654_-1.68142E+02
_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 4.115
_cell_length_b 10.636
_cell_length_c 21.213
_cell_angle_alpha 90.00
_cell_angle_beta 87.80
_cell_angle_gamma 90.00
_cell_volume 927.748
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.95886 0.75570 -0.59226
N2 N 0.78258 0.84210 -0.56020
H*3 H 0.64402 0.81880 -0.52161
H*4 H 0.78342 0.93312 -0.57379
N5 N 0.95104 0.63533 -0.57259
H*6 H 0.81237 0.61132 -0.53386
N7 N 1.14112 0.78645 -0.64304
H*8 H 1.15322 0.87567 -0.65922
H*9 H 1.26978 0.71739 -0.66556
N10 N 1.13569 0.54551 -0.60627
H*11 H 1.30238 0.50599 -0.57803
H*12 H 0.98802 0.47798 -0.62362
N'1+ N -0.38541 0.17483 0.45366
N'2+ N -0.12914 0.29755 0.38174
N3+ N -0.32752 0.29420 0.43319
N'4+ N -0.21958 0.09869 0.41430
C5+ C -0.06861 0.17368 0.37181
C6+ C 0.14192 0.13538 0.31914
N'7+ N 0.23967 0.02219 0.29909
N'8+ N 0.43674 0.04289 0.24718
N'9+ N 0.46466 0.16182 0.23447
N10+ N 0.28041 0.22130 0.27937

```
O11+ O -0.44839 0.39037 0.46000
H*12+ H 0.25549 0.31584 0.28145

#END

data_10647_-1.67925E+02
_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                 6.616
_cell_length_b                 20.125
_cell_length_c                 6.997
_cell_angle_alpha               90.00
_cell_angle_beta                75.42
_cell_angle_gamma                 90.00
_cell_volume                   901.628
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74315 0.66009 0.23096
N2 N 0.90175 0.70005 0.14434
H*3 H 1.04064 0.68146 0.06840
H*4 H 0.88672 0.74998 0.15263
N5 N 0.76957 0.59377 0.21642
H*6 H 0.90869 0.57478 0.14036
N7 N 0.56044 0.68459 0.33085
H*8 H 0.53470 0.73402 0.34499
H*9 H 0.44561 0.65214 0.39356
N10 N 0.60334 0.55228 0.30721
H*11 H 0.56072 0.52336 0.20443
H*12 H 0.64410 0.52332 0.41091
N'1+ N 0.31185 -0.15696 0.45115
N'2+ N 0.51175 -0.06566 0.39316
N3+ N 0.32205 -0.09016 0.47657
N'4+ N 0.50052 -0.17625 0.34827
C5+ C 0.61725 -0.12110 0.31524
C6+ C 0.83453 -0.11619 0.20914
N'7+ N 0.97180 -0.16197 0.11979
N'8+ N 1.15361 -0.12887 0.04424
N'9+ N 1.13513 -0.06574 0.08227
N10+ N 0.93508 -0.05697 0.18603
O11+ O 0.16902 -0.05561 0.56865
```

```
H*12+ H 0.87503 -0.01220 0.23642

#END

data_03538_-1.67678E+02
_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                 23.776
_cell_length_b                 3.939
_cell_length_c                 20.444
_cell_angle_alpha               90.00
_cell_angle_beta                74.54
_cell_angle_gamma                 90.00
_cell_volume                   1845.38
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.59642 0.91560 0.33952
N2 N 0.56665 0.76179 0.30075
H*3 H 0.52605 0.66955 0.32080
H*4 H 0.58404 0.73381 0.25028
N5 N 0.57167 0.94779 0.40660
H*6 H 0.53090 0.85569 0.42706
N7 N 0.64984 1.03690 0.31308
H*8 H 0.66983 1.01757 0.26302
H*9 H 0.67044 1.15105 0.34470
N10 N 0.60298 1.10869 0.44684
H*11 H 0.58120 1.31903 0.46922
H*12 H 0.60953 0.94564 0.48277
N'1+ N 0.04702 1.00105 0.15881
N'2+ N 0.10888 0.76212 0.06832
N3+ N 0.05910 0.93544 0.09117
N'4+ N 0.09027 0.86619 0.18036
C5+ C 0.12665 0.72509 0.12566
C6+ C 0.18035 0.54646 0.12297
N'7+ N 0.20725 0.47564 0.17085
N'8+ N 0.25634 0.30126 0.13920
```

N'9+ N 0.26089 0.26183 0.07498
N10+ N 0.21337 0.41486 0.06398
O11+ O 0.02674 1.02858 0.05452
H*12+ H 0.20515 0.42459 0.01794

#END

S24. Optimized crystal structure coordinates for 5 polymorphs of **3f** (ionic form).

data_01794_-1.61425E+02
_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 11.233
_cell_length_b 11.164
_cell_length_c 4.318
_cell_angle_alpha 71.54
_cell_angle_beta 71.84
_cell_angle_gamma 90.30
_cell_volume 484.797
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.14418 0.19906 0.42687
N2 N -0.24537 0.15200 0.38340
H*3 H -0.28947 0.21390 0.23930
N4 N -0.10558 0.32470 0.27987
H*5 H -0.02901 0.36123 0.31137
N6 N -0.08260 0.12240 0.61325
H*7 H -0.11499 0.02856 0.71899
H*8 H -0.00607 0.15536 0.65011
N9 N -0.17252 0.40246 0.08573
N10 N -0.28506 0.02129 0.53686
H*11 H -0.28196 -0.01766 0.35111
H*12 H -0.20838 0.46928 0.19252
H*13 H -0.11548 0.44512 -0.16328
H*14 H -0.37464 0.00645 0.70608
N'1+ N 0.14204 0.20281 0.69572
N'2+ N 0.23644 0.37222 0.73458
N3+ N 0.14227 0.32859 0.65654
N'4+ N 0.23892 0.16391 0.80225
C5+ C 0.29391 0.26628 0.82374
C6+ C 0.40347 0.27263 0.92846
N'7+ N 0.47629 0.18448 1.02699
N'8+ N 0.56583 0.24441 1.09542
N'9+ N 0.55183 0.36366 1.04443

N10+ N 0.44997 0.38289 0.93920
O11+ O 0.06230 0.39577 0.55761
H*12+ H 0.41628 0.46808 0.87971

#END

data_02228_-1.59119E+02
_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 13.203
_cell_length_b 7.604
_cell_length_c 7.351
_cell_angle_alpha 95.55
_cell_angle_beta 125.83
_cell_angle_gamma 111.94
_cell_volume 503.83
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.10705 0.23087 0.32437
N2 N -0.18042 0.22148 0.39715
H*3 H -0.27230 0.22800 0.28636
N4 N -0.15734 0.24833 0.11036
H*5 H -0.10249 0.25556 0.05370
N6 N 0.01415 0.22302 0.46217
H*7 H 0.04793 0.20986 0.62172
H*8 H 0.07155 0.22979 0.41168
N9 N -0.28504 0.25615 -0.02980
N10 N -0.12759 0.20333 0.61984
H*11 H -0.20544 0.06880 0.58699
H*12 H -0.26202 0.39349 -0.04770
H*13 H -0.36513 0.13360 -0.19943
H*14 H -0.10258 0.32808 0.73837
N'1+ N 0.17098 0.22017 0.31900
N'2+ N 0.24645 0.38261 0.14543
N3+ N 0.15974 0.34402 0.19517
N'4+ N 0.26782 0.17736 0.35030
C5+ C 0.31145 0.27563 0.24556
C6+ C 0.41639 0.27679 0.23141
N'7+ N 0.49456 0.18660 0.31294
N'8+ N 0.57533 0.24147 0.24748
N'9+ N 0.55097 0.35955 0.13111
N10+ N 0.45112 0.38321 0.11952

```
O11+ O 0.07660 0.41389 0.13481
H*12+ H 0.41092 0.46867 0.03809

#END

data_04190_-1.59073E+02
_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                 8.072
_cell_length_b                 13.068
_cell_length_c                 9.193
_cell_angle_alpha               142.04
_cell_angle_beta                77.99
_cell_angle_gamma                118.90
_cell_volume                   494.536
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.26283 0.28497 0.35781
N2 N 0.31538 0.28874 0.49144
H*3 H 0.41842 0.25281 0.45381
N4 N 0.34752 0.23443 0.18156
H*5 H 0.30865 0.23116 0.07939
N6 N 0.12844 0.33069 0.39899
H*7 H 0.06864 0.36781 0.53341
H*8 H 0.08614 0.32904 0.30099
N9 N 0.48819 0.18728 0.14329
N10 N 0.22681 0.34140 0.67443
H*11 H 0.33382 0.46337 0.84501
H*12 H 0.43975 0.04663 -0.03447
H*13 H 0.62251 0.28172 0.17718
H*14 H 0.15150 0.22884 0.63385
N'1+ N 0.03714 0.69924 -0.10799
N'2+ N 0.06309 0.86323 0.27538
N3+ N -0.00917 0.81992 0.10440
N'4+ N 0.14248 0.66342 -0.07342
C5+ C 0.15624 0.76248 0.15612
C6+ C 0.25675 0.77026 0.28012
N'7+ N 0.35773 0.68681 0.20674
N'8+ N 0.41962 0.74570 0.40044
N'9+ N 0.36236 0.85989 0.58709
N10+ N 0.25962 0.87677 0.51420
O11+ O -0.10910 0.88314 0.13502
```

```
H*12+ H 0.19648 0.95798 0.62306

#END

data_07363_-1.58962E+02
_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                 10.135
_cell_length_b                 7.377
_cell_length_c                 8.800
_cell_angle_alpha               83.67
_cell_angle_beta                91.78
_cell_angle_gamma               50.20
_cell_volume                   497.932
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.33831 0.15701 -0.38729
N2 N 0.26615 0.08065 -0.45596
H*3 H 0.18424 0.18235 -0.55562
N4 N 0.29989 0.36256 -0.45223
H*5 H 0.35392 0.42185 -0.40104
N6 N 0.44670 0.03100 -0.25640
H*7 H 0.47185 -0.12250 -0.21171
H*8 H 0.50288 0.08444 -0.20224
N9 N 0.18547 0.49041 -0.58980
N10 N 0.30659 -0.13320 -0.38789
H*11 H 0.36302 -0.25331 -0.46184
H*12 H 0.07923 0.65654 -0.57430
H*13 H 0.24581 0.50347 -0.67524
H*14 H 0.19682 -0.10060 -0.36114
N'1+ N 0.60363 0.18039 -0.10289
N'2+ N 0.71874 0.35327 -0.15713
N3+ N 0.62226 0.30433 -0.21313
N'4+ N 0.69062 0.14818 0.02831
C5+ C 0.75822 0.25252 -0.00652
C6+ C 0.86397 0.26569 0.09765
N'7+ N 0.92074 0.18344 0.24801
N'8+ N 1.01518 0.24815 0.28505
N'9+ N 1.01923 0.36476 0.16629
N10+ N 0.92459 0.37727 0.04738
O11+ O 0.55558 0.36547 -0.35223
H*12+ H 0.90483 0.45909 -0.06119
```

```
#END

data_01502_-1.58705E+02
_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                 12.017
_cell_length_b                 10.873
_cell_length_c                 3.951
_cell_angle_alpha               80.71
_cell_angle_beta                79.09
_cell_angle_gamma               101.68
_cell_volume                   485.586
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.18095 0.19979 0.32042
N2 N -0.28935 0.15489 0.28393
H*3 H -0.32813 0.21814 0.16096
N4 N -0.12853 0.32514 0.19442
H*5 H -0.04641 0.36003 0.22085
N6 N -0.12581 0.12130 0.47944
H*7 H -0.16860 0.02775 0.57011
H*8 H -0.04410 0.15260 0.51045
N9 N -0.18905 0.40486 0.02880
N10 N -0.34341 0.02448 0.41547
H*11 H -0.36323 -0.01793 0.21558
H*12 H -0.19985 0.47605 0.16147
H*13 H -0.14532 0.44318 -0.22566
H*14 H -0.41763 0.01487 0.60180
N'1+ N 0.10251 0.19758 0.58342
N'2+ N 0.21832 0.36797 0.69567
N3+ N 0.11985 0.32414 0.59611
N'4+ N 0.19242 0.15836 0.67754
C5+ C 0.26038 0.26132 0.74329
C6+ C 0.36891 0.26761 0.85473
N'7+ N 0.42848 0.17885 0.91964
N'8+ N 0.52463 0.23908 1.01613
N'9+ N 0.52709 0.35908 1.01378
N10+ N 0.42961 0.37852 0.91267
O11+ O 0.05041 0.39181 0.52189
H*12+ H 0.40810 0.46427 0.88705
```

#END
S26. Optimized crystal structure coordinates for 5 polymorphs of **3g** (ionic form).
data_05426_-1.53295E+02
_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 8.307
_cell_length_b 18.977
_cell_length_c 10.146
_cell_angle_alpha 90.00
_cell_angle_beta 138.92
_cell_angle_gamma 90.00
_cell_volume 1051.01
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.01142 0.68207 -0.09535
N2 N 0.01884 0.63177 -0.16801
H*3 H -0.03630 0.64271 -0.29552
N4 N 0.05820 0.67036 0.07242
H*5 H 0.13314 0.62267 0.14004
N6 N -0.11130 0.74408 -0.19046
H*7 H -0.13110 0.78083 -0.13057
N8 N 0.02460 0.72379 0.14530
N9 N 0.12368 0.56741 -0.06582
H*10 H 0.28092 0.55900 -0.02047
H*11 H -0.08801 0.70654 0.14904
H*12 H 0.18919 0.73817 0.28574
H*13 H 0.00372 0.52737 -0.15717
N14 N -0.18254 0.75501 -0.36553
H*15 H -0.36577 0.76485 -0.48297
H*16 H -0.08857 0.79649 -0.34627
N'1+ N 0.35911 0.85102 0.36139
N'2+ N 0.14003 0.94844 0.18534
N3+ N 0.21788 0.88656 0.18606
N'4+ N 0.37305 0.89109 0.47754
C5+ C 0.24129 0.94888 0.36984
C6+ C 0.20056 1.00838 0.43097
N'7+ N 0.27715 1.02191 0.60047
N'8+ N 0.18241 1.08595 0.57404
N'9+ N 0.05289 1.11216 0.39873
N10+ N 0.06255 1.06392 0.30684

```
O11+ O 0.16702 0.86335 0.04125
H*12+ H -0.02273 1.07017 0.16647

#END

data_10383_-1.53191E+02
_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                 15.296
_cell_length_b                 7.126
_cell_length_c                 11.549
_cell_angle_alpha               90.00
_cell_angle_beta                120.09
_cell_angle_gamma                90.00
_cell_volume                   1089.19
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.27320 0.39817 0.62643
N2 N 0.25507 0.50830 0.70618
H*3 H 0.18361 0.50995 0.69099
N4 N 0.36614 0.39082 0.64222
H*5 H 0.42077 0.47085 0.71577
N6 N 0.19839 0.29539 0.53089
H*7 H 0.21522 0.21372 0.47253
N8 N 0.38314 0.27462 0.55758
N9 N 0.33454 0.61434 0.80528
H*10 H 0.34670 0.57694 0.89731
H*11 H 0.40707 0.35281 0.50494
H*12 H 0.43622 0.17621 0.61254
H*13 H 0.31754 0.75354 0.78971
N14 N 0.10192 0.30555 0.51643
H*15 H 0.05126 0.35305 0.42324
H*16 H 0.08042 0.17646 0.53084
N'1+ N 0.07339 -0.00920 -0.17675
N'2+ N 0.21665 -0.01884 -0.18481
N3+ N 0.11563 -0.02314 -0.25570
N'4+ N 0.14932 0.00453 -0.05107
C5+ C 0.23400 -0.00150 -0.05808
C6+ C 0.33669 0.00844 0.05236
N'7+ N 0.37408 0.02529 0.18393
```

N'8+ N 0.47630 0.02733 0.23972
N'9+ N 0.50329 0.01274 0.15001
N10+ N 0.41622 0.00071 0.03151
O11+ O 0.06468 -0.03836 -0.38153
H*12+ H 0.41377 -0.01202 -0.05732

#END

data_01266_-1.53029E+02
_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 10.420
_cell_length_b 14.672
_cell_length_c 7.676
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1173.52
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.48697 -0.24088 0.48452
N2 N 0.48555 -0.25151 0.31107
H*3 H 0.47282 -0.19485 0.23682
N4 N 0.50344 -0.31339 0.58843
H*5 H 0.51451 -0.37523 0.53064
N6 N 0.47192 -0.15775 0.55406
H*7 H 0.47358 -0.15256 0.68610
N8 N 0.50456 -0.30047 0.76930
N9 N 0.50148 -0.33911 0.24162
H*10 H 0.58096 -0.34088 0.16448
H*11 H 0.43219 -0.33679 0.82526
H*12 H 0.59034 -0.32099 0.81933
H*13 H 0.42281 -0.35668 0.17041
N14 N 0.45487 -0.08306 0.44264
H*15 H 0.36868 -0.05287 0.46678
H*16 H 0.52684 -0.03707 0.46085
N'1+ N -0.22221 0.53057 0.03670
N'2+ N -0.07996 0.64299 -0.00504
N3+ N -0.20422 0.62125 0.00932
N'4+ N -0.10616 0.49251 0.04016

```
C5+ C -0.02277 0.56065 0.01504
C6+ C 0.11556 0.55391 0.00801
N'7+ N 0.19451 0.48281 0.02343
N'8+ N 0.31527 0.51679 0.00576
N'9+ N 0.31448 0.60423 -0.01947
N10+ N 0.18941 0.62862 -0.01839
O11+ O -0.29509 0.67797 -0.00117
H*12+ H 0.15914 0.69354 -0.03519

#END

data_02215_-1.52870E+02
_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                 16.306
_cell_length_b                 13.786
_cell_length_c                 10.354
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   2327.52
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.64908 0.75869 0.76594
N2 N 0.68579 0.67211 0.75447
H*3 H 0.74810 0.67092 0.75177
N4 N 0.56704 0.76433 0.76996
H*5 H 0.53489 0.70132 0.76403
N6 N 0.69441 0.83963 0.77339
H*7 H 0.66425 0.90383 0.78202
N8 N 0.53015 0.85570 0.78199
N9 N 0.63704 0.58859 0.74686
H*10 H 0.65017 0.54337 0.82184
H*11 H 0.49350 0.86878 0.70428
H*12 H 0.49615 0.85839 0.86442
H*13 H 0.64751 0.55376 0.66170
```

N14 N 0.78004 0.83178 0.76897
H*15 H 0.80225 0.86911 0.69163
H*16 H 0.80490 0.85872 0.85177
N'1+ N 0.91659 -0.11812 0.48814
N'2+ N 0.83392 -0.04779 0.34285
N3+ N 0.84704 -0.06577 0.46815
N'4+ N 0.94942 -0.13450 0.37236
C5+ C 0.89923 -0.09200 0.28714
C6+ C 0.90852 -0.08957 0.14830
N'7+ N 0.96579 -0.12640 0.07049
N'8+ N 0.94311 -0.10162 -0.05155
N'9+ N 0.87551 -0.05196 -0.05261
N10+ N 0.85297 -0.04376 0.07253
O11+ O 0.80054 -0.03766 0.55824
H*12+ H 0.80191 -0.00824 0.10156

#END

data_01226_-1.52740E+02
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P n a 21'
_symmetry_Int_Tables_number 33
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,1/2+z
3 1/2+x,1/2-y,z
4 -x,-y,1/2+z
_cell_length_a 10.473
_cell_length_b 14.748
_cell_length_c 7.616
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1176.34
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.26365 0.24080 0.60000
N2 N 0.26500 0.24629 0.42431
H*3 H 0.27571 0.18767 0.35567
N4 N 0.24979 0.31608 0.69679
H*5 H 0.24060 0.37599 0.63201
N6 N 0.27616 0.16003 0.67889
H*7 H 0.27465 0.15874 0.81232
N8 N 0.24868 0.30853 0.88019
N9 N 0.25176 0.33152 0.34503
H*10 H 0.17258 0.33230 0.26743

H*11 H 0.32194 0.34507 0.93241
H*12 H 0.16412 0.33174 0.92855
H*13 H 0.33039 0.34563 0.27129
N14 N 0.29051 0.08235 0.57478
H*15 H 0.37534 0.05169 0.60210
H*16 H 0.21753 0.03836 0.59824
N'1+ N 0.02399 0.52908 -0.37709
N'2+ N 0.16673 0.64181 -0.39603
N3+ N 0.04280 0.62012 -0.38879
N'4+ N 0.13916 0.49073 -0.37675
C5+ C 0.22286 0.55907 -0.38813
C6+ C 0.36053 0.55215 -0.39242
N'7+ N 0.43843 0.48067 -0.38669
N'8+ N 0.55900 0.51466 -0.39529
N'9+ N 0.55907 0.60247 -0.40590
N10+ N 0.43479 0.62710 -0.40424
O11+ O -0.04712 0.67717 -0.39233
H*12+ H 0.40529 0.69232 -0.41102

#END

S27. Optimized crystal structure coordinates for 5 polymorphs of **4a** (ionic form).

data_07603_-1.69448E+02
_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 6.334
_cell_length_b 8.559
_cell_length_c 14.616
_cell_angle_alpha 90.00
_cell_angle_beta 109.94
_cell_angle_gamma 90.00
_cell_volume 744.87
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.47462 -0.12762 0.65892
H*2 H 0.35949 -0.15438 0.69190
H*3 H 0.63305 -0.12590 0.71023
H*4 H 0.46771 -0.21048 0.60707
H*5 H 0.43824 -0.01972 0.62647
N'1+ N -0.30417 0.64412 -0.05405
N2+ N -0.02381 0.78214 0.01921

N'3+ N -0.09904 0.67555 -0.05060
N'4+ N -0.36247 0.72825 0.01207
C5+ C -0.18407 0.81630 0.05885
C6+ C -0.13582 0.92955 0.13599
N7+ N -0.26325 0.98426 0.18737
N'8+ N -0.13447 1.09082 0.25214
N'9+ N 0.06155 1.09835 0.23921
N'10+ N 0.06640 1.00142 0.16887
O11+ O 0.18772 0.84228 0.04275
O12+ O -0.46299 0.94867 0.18043
H*13+ H 0.19478 0.91857 0.09710

#END

data_00372_-1.69360E+02
_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 7.127
_cell_length_b 5.581
_cell_length_c 8.880
_cell_angle_alpha 90.88
_cell_angle_beta 77.66
_cell_angle_gamma 98.37
_cell_volume 341.328
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.36013 0.50491 -0.23117
H*2 H 0.47456 0.61214 -0.19907
H*3 H 0.24018 0.59267 -0.20872
H*4 H 0.39602 0.47066 -0.34705
H*5 H 0.32976 0.34417 -0.16984
N'1+ N 0.30424 0.12029 -0.01588
N2+ N 0.16936 -0.17234 0.13268
N'3+ N 0.20287 -0.09596 -0.01306
N'4+ N 0.33664 0.18462 0.12497
C5+ C 0.25082 -0.00157 0.21984
C6+ C 0.23107 -0.04917 0.38165
N7+ N 0.29690 0.08746 0.49289
N'8+ N 0.23662 -0.04562 0.62683
N'9+ N 0.13888 -0.25296 0.59527
N'10+ N 0.13271 -0.26110 0.44667
O11+ O 0.06589 -0.39448 0.17779

```
O12+ O 0.39542 0.29788 0.48256
H*13+ H 0.06531 -0.39960 0.29238

#END

data_05801_-1.69207E+02
_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                 6.335
_cell_length_b                 12.582
_cell_length_c                 9.012
_cell_angle_alpha               90.00
_cell_angle_beta                100.05
_cell_angle_gamma               90.00
_cell_volume                   707.297
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.00169 -0.05434 -0.24692
H*2 H -0.03485 0.01767 -0.20387
H*3 H -0.12724 -0.10470 -0.25271
H*4 H 0.03670 -0.04348 -0.35304
H*5 H 0.13216 -0.08685 -0.17806
N'1+ N 0.31555 0.88905 -0.00302
N2+ N 0.58072 0.86456 0.16847
N'3+ N 0.52237 0.87061 0.01962
N'4+ N 0.23964 0.89499 0.12813
C5+ C 0.40832 0.87941 0.23758
C6+ C 0.43747 0.87586 0.39942
N7+ N 0.29532 0.88788 0.49510
N'8+ N 0.40916 0.87695 0.63768
N'9+ N 0.61094 0.85916 0.62604
N'10+ N 0.63383 0.85799 0.48218
O11+ O 0.78889 0.84574 0.23280
O12+ O 0.09485 0.90580 0.46569
H*13+ H 0.78215 0.84567 0.34478

#END

data_04481_-1.69098E+02
_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                   5.511
_cell_length_b                   8.888
_cell_length_c                   14.066
_cell_angle_alpha                 90.00
_cell_angle_beta                  99.00
_cell_angle_gamma                    90.00
_cell_volume                     680.495
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.51220 0.30946 0.67118
H*2 H -0.68250 0.35932 0.65896
H*3 H -0.53227 0.19491 0.67633
H*4 H -0.41922 0.33366 0.61515
H*5 H -0.41481 0.34995 0.73428
N'1+ N 0.09220 0.98812 0.14925
N2+ N -0.19576 0.84960 0.08521
N'3+ N -0.13094 0.99273 0.10064
N'4+ N 0.17227 0.84504 0.16542
C5+ C -0.01092 0.75656 0.12467
C6+ C -0.04445 0.59636 0.11591
N7+ N 0.10744 0.48042 0.14799
N'8+ N -0.01709 0.35103 0.11966
N'9+ N -0.23435 0.38971 0.07264
N'10+ N -0.25712 0.53862 0.06902
O11+ O -0.42090 0.81211 0.03578
O12+ O 0.32383 0.48352 0.19520
H*13+ H -0.41512 0.69768 0.03600

#END

data_02024_-1.69014E+02
_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 9.509
_cell_length_b 13.502
_cell_length_c 5.188
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 666.09
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.50004 -0.44724 -0.52456
H*2 H 0.47087 -0.38393 -0.62068
H*3 H 0.42662 -0.46332 -0.38533
H*4 H 0.50622 -0.50509 -0.65283
H*5 H 0.59646 -0.43662 -0.43940
N'1+ N 0.27481 0.91104 -0.00598
N2+ N 0.29708 0.75695 -0.03632
N'3+ N 0.33429 0.84199 -0.14622
N'4+ N 0.20013 0.87221 0.19181
C5+ C 0.21417 0.77402 0.17288
C6+ C 0.16243 0.69127 0.31956
N7+ N 0.07940 0.68754 0.53264
N'8+ N 0.06282 0.58964 0.59196
N'9+ N 0.13363 0.53779 0.41976
N'10+ N 0.19568 0.59751 0.25069
O11+ O 0.34120 0.66832 -0.13389
O12+ O 0.02458 0.75791 0.66074
H*13+ H 0.29655 0.61869 -0.01107

#END

S28. Optimized crystal structure coordinates for 5 polymorphs of **4b** (ionic form).

data_04012_-1.77026E+02
_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 7.253
_cell_length_b 5.448
_cell_length_c 8.793
_cell_angle_alpha 91.77
_cell_angle_beta 99.90
_cell_angle_gamma 86.47
_cell_volume 341.554

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.15352 0.44797 -0.23967
H*2 H 0.20746 0.26978 -0.22156
H*3 H 0.25466 0.56699 -0.19269
H*4 H 0.11469 0.47348 -0.35699
O5 O -0.00200 0.46808 -0.16327
H*6 H -0.05758 0.63540 -0.17768
N'1+ N 0.22996 1.03129 -0.03705
N2+ N 0.34607 0.77110 0.12859
N'3+ N 0.32483 0.81828 -0.02112
N'4+ N 0.18972 1.12212 0.09925
C5+ C 0.26357 0.95663 0.20498
C6+ C 0.27079 0.94100 0.36894
N7+ N 0.20127 1.09748 0.47137
N'8+ N 0.24844 0.99203 0.61278
N'9+ N 0.34232 0.78114 0.59395
N'10+ N 0.35849 0.74431 0.44652
O11+ O 0.43996 0.56046 0.18698
O12+ O 0.10959 1.30328 0.44832
H*13+ H 0.43250 0.57762 0.30135

#END

data_00021_-1.76246E+02
_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                 13.273
_cell_length_b                 9.604
_cell_length_c                 8.754
_cell_angle_alpha               90.00
_cell_angle_beta                42.26
_cell_angle_gamma                 90.00
_cell_volume                   750.443
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

N1 N 0.92501 0.49244 -0.16849
H*2 H 0.97568 0.39865 -0.24995
H*3 H 0.81257 0.48557 -0.06921
H*4 H 0.93936 0.51387 -0.06989
O5 O 0.99959 0.58973 -0.34502
H*6 H 0.95467 0.68066 -0.27464
N'1+ N 0.09457 0.18674 0.40468
N2+ N 0.17968 0.04730 0.47187
N'3+ N 0.16619 0.06817 0.33744
N'4+ N 0.06171 0.24258 0.57951
C5+ C 0.11584 0.15391 0.62264
C6+ C 0.11845 0.15122 0.78399
N7+ N 0.06399 0.24254 0.94996
N'8+ N 0.09728 0.18877 1.05306
N'9+ N 0.16874 0.07011 0.95116
N'10+ N 0.18356 0.04406 0.78613
O11+ O 0.24981 -0.06837 0.44894
O12+ O -0.00508 0.35681 1.00709
H*13+ H 0.24217 -0.05455 0.57249

#END

data_01269_-1.75271E+02
_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 8.776
_cell_length_b 5.425
_cell_length_c 7.308
_cell_angle_alpha 93.51
_cell_angle_beta 92.81
_cell_angle_gamma 91.47
_cell_volume 346.719
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.74194 0.45651 0.84691
H*2 H 0.72835 0.27556 0.79572
H*3 H 0.85605 0.49269 0.88253
H*4 H 0.70372 0.57090 0.74753
O5 O 0.65209 0.47156 1.00105
H*6 H 0.66185 0.64129 1.05401
N'1+ N 0.53985 -0.00069 0.77433
N2+ N 0.36800 -0.24492 0.65679

N'3+ N 0.51865 -0.21263 0.67914
N'4+ N 0.40601 0.10401 0.81367
C5+ C 0.29632 -0.05129 0.73891
C6+ C 0.13222 -0.05055 0.73050
N7+ N 0.03383 0.11658 0.79943
N'8+ N -0.10999 0.02503 0.75114
N'9+ N -0.09643 -0.18825 0.65722
N'10+ N 0.04986 -0.23994 0.64206
O11+ O 0.30446 -0.45022 0.56229
O12+ O 0.06195 0.32056 0.89146
H*13+ H 0.19068 -0.42157 0.56895

#END

data_10925_-1.75251E+02
_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 10.836
_cell_length_b 8.809
_cell_length_c 7.439
_cell_angle_alpha 90.00
_cell_angle_beta 91.41
_cell_angle_gamma 90.00
_cell_volume 709.87
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.02105 0.75747 -0.14628
H*2 H -0.10870 0.74618 -0.20164
H*3 H 0.04203 0.72023 -0.23835
H*4 H -0.00605 0.87019 -0.11436
O5 O -0.02101 0.66528 0.00799
H*6 H 0.06096 0.67279 0.06485
N'1+ N 0.77346 0.55149 -0.23812
N2+ N 0.64463 0.39464 -0.34167
N'3+ N 0.66800 0.54243 -0.32767
N'4+ N 0.81841 0.41265 -0.19421
C5+ C 0.73647 0.31250 -0.26006
C6+ C 0.72871 0.14948 -0.26014
N7+ N 0.80617 0.04231 -0.18979
N'8+ N 0.75395 -0.09534 -0.22880

N'9+ N 0.64955 -0.06980 -0.31884
N'10+ N 0.63133 0.07841 -0.34033
O11+ O 0.54035 0.34316 -0.42853
O12+ O 0.90805 0.05871 -0.10357
H*13+ H 0.54882 0.22854 -0.41670

#END

data_06967_-1.75082E+02
_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 12.908
_cell_length_b 6.783
_cell_length_c 8.801
_cell_angle_alpha 90.00
_cell_angle_beta 84.06
_cell_angle_gamma 90.00
_cell_volume 766.434
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.51769 0.08608 0.73019
H*2 H 0.59276 0.07717 0.67787
H*3 H 0.47555 -0.03240 0.69585
H*4 H 0.51993 0.08476 0.84718
O5 O 0.47965 0.26609 0.67946
H*6 H 0.40818 0.28036 0.72671
N'1+ N 0.30800 0.88446 -0.51567
N2+ N 0.18421 0.84392 -0.34456
N'3+ N 0.20657 0.86345 -0.49474
N'4+ N 0.35136 0.87885 -0.38213
C5+ C 0.27263 0.85302 -0.27291
C6+ C 0.26530 0.83491 -0.10929
N7+ N 0.33989 0.83872 -0.01103
N'8+ N 0.28978 0.81473 0.13227
N'9+ N 0.18934 0.79746 0.11854
N'10+ N 0.17169 0.80911 -0.02737
O11+ O 0.08395 0.81881 -0.28141
O12+ O 0.43788 0.85979 -0.03888
H*13+ H 0.09220 0.80873 -0.16794

#END

S29. Optimized crystal structure coordinates for 5 polymorphs of **4c** (ionic form).

```
data_00813_-1.70151E+02
_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                 8.286
_cell_length_b                 12.468
_cell_length_c                 11.302
_cell_angle_alpha               39.71
_cell_angle_beta                83.26
_cell_angle_gamma                50.49
_cell_volume                   377.515
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.82963 0.99057 0.34599
H*2 H 0.87987 0.97992 0.43651
H*3 H 0.66563 1.04051 0.32214
N4 N 1.11868 0.66791 0.54233
H*5 H 1.06594 0.67959 0.45226
H*6 H 1.28140 0.61865 0.56728
H*7 H 0.72668 1.18307 0.14876
N'1+ N -0.34562 0.40775 -0.27789
N2+ N -0.00534 0.29531 -0.18790
N'3+ N -0.17923 0.37231 -0.32013
N'4+ N -0.28241 0.35517 -0.12129
C5+ C -0.06562 0.28347 -0.06368
C6+ C 0.09921 0.20386 0.09089
N7+ N 0.08399 0.17590 0.23246
N'8+ N 0.29154 0.09519 0.34087
N'9+ N 0.42381 0.07647 0.26554
N'10+ N 0.31178 0.14139 0.11278
O11+ O 0.19916 0.24009 -0.18838
O12+ O -0.08394 0.21377 0.26585
H*13+ H 0.29419 0.18823 -0.07295

#END

data_06481_-1.69962E+02
_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                 5.158
_cell_length_b                 15.477
_cell_length_c                 9.330
_cell_angle_alpha               90.00
_cell_angle_beta                95.75
_cell_angle_gamma                 90.00
_cell_volume                   741.07
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.34482 0.27034 0.43624
H*2 H -0.26439 0.24828 0.34657
H*3 H -0.47074 0.22311 0.46416
N4 N -0.49587 0.34699 0.39592
H*5 H -0.57740 0.36791 0.48507
H*6 H -0.36988 0.39323 0.36681
H*7 H -0.19823 0.27764 0.51922
N'1+ N 1.20368 0.42248 -0.40381
N2+ N 0.90274 0.42085 -0.26844
N'3+ N 1.02417 0.37228 -0.35848
N'4+ N 1.20027 0.50232 -0.34483
C5+ C 1.00865 0.50144 -0.25851
C6+ C 0.90452 0.56423 -0.16609
N7+ N 0.97262 0.64772 -0.13693
N'8+ N 0.80915 0.67739 -0.04141
N'9+ N 0.65077 0.61356 -0.01547
N'10+ N 0.70364 0.54355 -0.08983
O11+ O 0.70141 0.38862 -0.20028
O12+ O 1.15032 0.69310 -0.18492
H*13+ H 0.65125 0.43989 -0.14063

#END

data_07251_-1.69826E+02
_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                 12.365
_cell_length_b                 11.450
_cell_length_c                 9.256
_cell_angle_alpha               90.00
_cell_angle_beta                37.04
_cell_angle_gamma                 90.00
_cell_volume                   789.383
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.57990 0.53219 0.66083
H*2 H 0.54504 0.55563 0.59444
H*3 H 0.54692 0.60160 0.76138
N4 N 0.77282 0.51704 0.46003
H*5 H 0.80653 0.49507 0.52757
H*6 H 0.80464 0.44885 0.35967
H*7 H 0.50402 0.46077 0.77202
N'1+ N 0.07556 0.80151 -0.11108
N2+ N 0.13144 0.65049 -0.05056
N'3+ N 0.11829 0.69102 -0.17077
N'4+ N 0.06096 0.83289 0.04499
C5+ C 0.09650 0.73680 0.08383
C6+ C 0.10375 0.71081 0.22805
N7+ N 0.07525 0.77943 0.37608
N'8+ N 0.09977 0.71006 0.46841
N'9+ N 0.14119 0.60449 0.37773
N'10+ N 0.14479 0.60188 0.23032
O11+ O 0.17476 0.53655 -0.07067
O12+ O 0.03378 0.88701 0.42675
H*13+ H 0.17424 0.53274 0.03971

#END

data_01139_-1.69752E+02
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,z
3 x,1/2-y,1/2+z
4 1/2-x,-y,1/2+z
5 -x,-y,-z
6 1/2+x,1/2-y,-z
7 -x,1/2+y,1/2-z
8 1/2+x,y,1/2-z
```

```
_cell_length_a                 7.101
_cell_length_b                 11.468
_cell_length_c                 19.098
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1555.23
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.13531 0.44946 0.60244
H*2 H -0.09557 0.39445 0.56255
H*3 H -0.15328 0.39836 0.64620
N4 N -0.31589 0.49982 0.58437
H*5 H -0.35532 0.55327 0.62458
H*6 H -0.29728 0.54934 0.54045
H*7 H -0.02740 0.50781 0.61176
N'1+ N 0.39084 0.28799 0.00827
N2+ N 0.31750 0.17454 0.08997
N'3+ N 0.33039 0.18196 0.02064
N'4+ N 0.41710 0.34892 0.06818
C5+ C 0.37045 0.27681 0.12032
C6+ C 0.36656 0.28691 0.19538
N7+ N 0.41135 0.37734 0.23828
N'8+ N 0.38188 0.33952 0.30523
N'9+ N 0.32192 0.23075 0.30172
N'10+ N 0.31096 0.19591 0.23544
O11+ O 0.25787 0.07437 0.12162
O12+ O 0.46972 0.47894 0.22284
H*13+ H 0.26313 0.09562 0.17331

#END

data_02288_-1.69624E+02
_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                 7.632
_cell_length_b                 10.995
_cell_length_c                 9.090
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
```

```
_cell_angle_gamma              90.00
_cell_volume                  762.777
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.34777 -0.03484 -0.19396
H*2 H 0.37669 -0.07547 -0.09495
H*3 H 0.26521 -0.09312 -0.24901
N4 N 0.50856 -0.02480 -0.27766
H*5 H 0.47841 0.01435 -0.37640
H*6 H 0.59053 0.03211 -0.22147
H*7 H 0.28198 0.04554 -0.17387
N'1+ N 0.75571 0.28685 -0.09769
N2+ N 0.66076 0.13502 0.01699
N'3+ N 0.71054 0.17278 -0.11558
N'4+ N 0.73604 0.32327 0.04360
C5+ C 0.67555 0.22666 0.11689
C6+ C 0.62794 0.20438 0.26763
N7+ N 0.63007 0.27843 0.38738
N'8+ N 0.57138 0.21054 0.50323
N'9+ N 0.53607 0.10057 0.45319
N'10+ N 0.56912 0.09367 0.30982
O11+ O 0.60449 0.01858 0.03911
O12+ O 0.67580 0.38929 0.39751
H*13+ H 0.57666 0.01788 0.14858

#END
```

S30. Optimized crystal structure coordinates for 5 polymorphs of **4d** (ionic form).

```
data_10533_-1.61200E+02
_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                 4.140
_cell_length_b                 12.385
_cell_length_c                 20.295
_cell_angle_alpha               90.00
_cell_angle_beta                57.79
_cell_angle_gamma              90.00
_cell_volume                  880.455
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74396 0.58891 0.18793
N2 N 0.79041 0.58187 0.11762
H*3 H 0.68383 0.63868 0.09855
H*4 H 0.93346 0.51954 0.08149
N5 N 0.55335 0.67231 0.23453
H*6 H 0.51498 0.67919 0.28787
H*7 H 0.44213 0.73089 0.21776
N8 N 0.88811 0.51254 0.21165
H*9 H 1.03307 0.44886 0.17736
H*10 H 0.85630 0.51629 0.26454
N'1+ N 0.73228 0.15484 -0.17283
N2+ N 0.79456 0.09585 -0.08333
N'3+ N 0.87082 0.07333 -0.15433
N'4+ N 0.56851 0.22932 -0.11523
C5+ C 0.60784 0.19191 -0.05813
C6+ C 0.49891 0.23111 0.01773
N7+ N 0.31363 0.32267 0.05638
N'8+ N 0.28453 0.31938 0.12664
N'9+ N 0.44700 0.22908 0.12912
N'10+ N 0.58084 0.17329 0.06359
O11+ O 0.90036 0.02708 -0.04553
O12+ O 0.18538 0.39929 0.03500
H*13+ H 0.80459 0.06575 0.00592

#END

data_04097_-1.60969E+02
_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                 3.927
_cell_length_b                 10.275
_cell_length_c                 22.873
_cell_angle_alpha               90.00
_cell_angle_beta                102.15
_cell_angle_gamma                90.00
_cell_volume                   902.25
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

```
_atom_site_fract_z
C1 C -0.08716 0.28741 0.40509
N2 N -0.29531 0.29760 0.35091
H*3 H -0.32712 0.38335 0.32879
H*4 H -0.42688 0.21986 0.33051
N5 N 0.08381 0.39194 0.43102
H*6 H 0.24237 0.38639 0.47193
H*7 H 0.05943 0.47953 0.41047
N8 N -0.04997 0.17269 0.43334
H*9 H -0.17673 0.09250 0.41455
H*10 H 0.10597 0.16284 0.47429
N'1+ N -0.34554 0.94600 -0.21539
N2+ N -0.11812 0.76333 -0.22193
N'3+ N -0.33893 0.84938 -0.25257
N'4+ N -0.13364 0.92392 -0.16149
C5+ C 0.01158 0.80757 -0.16554
C6+ C 0.25633 0.72849 -0.12498
N7+ N 0.42273 0.74900 -0.06732
N'8+ N 0.62635 0.64212 -0.05022
N'9+ N 0.58098 0.56177 -0.09622
N'10+ N 0.35677 0.61147 -0.14259
O11+ O -0.04761 0.64893 -0.24735
O12+ O 0.40485 0.84574 -0.03344
H*13+ H 0.12540 0.60557 -0.21360

#END

data_05279_-1.60853E+02
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z
_cell_length_a                 19.025
_cell_length_b                 4.029
_cell_length_c                 24.754
_cell_angle_alpha               90.00
_cell_angle_beta                67.32
_cell_angle_gamma                 90.00
_cell_volume                   1750.71
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.40314 0.81042 0.40117
N2 N 0.34530 0.61102 0.43184
H*3 H 0.33494 0.55096 0.47386
H*4 H 0.31025 0.51457 0.41389
N5 N 0.44861 0.93452 0.42605
H*6 H 0.49264 1.08564 0.40366
H*7 H 0.44028 0.88080 0.46795
N8 N 0.41551 0.88572 0.34562
H*9 H 0.38184 0.79466 0.32599
H*10 H 0.45888 1.03588 0.32167
N'1+ N 0.55097 -0.32828 -0.21752
N2+ N 0.64339 -0.62377 -0.22103
N'3+ N 0.60364 -0.52705 -0.25219
N'4+ N 0.55601 -0.29511 -0.16472
C5+ C 0.61487 -0.48318 -0.16685
C6+ C 0.65002 -0.55645 -0.12615
N7+ N 0.63326 -0.45157 -0.07035
N'8+ N 0.68500 -0.59811 -0.05204
N'9+ N 0.73049 -0.78241 -0.09556
N'10+ N 0.71073 -0.76265 -0.14145
O11+ O 0.70367 -0.83568 -0.24399
O12+ O 0.58091 -0.25678 -0.03890
H*13+ H 0.72165 -0.86137 -0.21047

#END

data_00697_-1.60044E+02
_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                 3.960
_cell_length_b                 10.130
_cell_length_c                 14.214
_cell_angle_alpha               111.90
_cell_angle_beta                58.60
_cell_angle_gamma                92.92
_cell_volume                   444.103
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.83706 -0.30474 -0.19076
```

N2 N 0.55453 -0.18578 -0.12610
H*3 H 0.57522 -0.10977 -0.15804
H*4 H 0.31208 -0.16841 -0.04341
N5 N 1.15477 -0.32490 -0.29996
H*6 H 1.37167 -0.41400 -0.35031
H*7 H 1.18722 -0.25162 -0.33531
N8 N 0.80189 -0.40354 -0.14622
H*9 H 0.56429 -0.39044 -0.06393
H*10 H 1.01188 -0.49419 -0.19356
N'1+ N 0.76568 0.39763 0.55939
N2+ N 0.99560 0.21338 0.55672
N'3+ N 1.07499 0.29151 0.49265
N'4+ N 0.48901 0.38941 0.66505
C5+ C 0.63485 0.27207 0.66356
C6+ C 0.49284 0.20345 0.74648
N7+ N 0.15013 0.23875 0.85708
N'8+ N 0.16817 0.13632 0.89607
N'9+ N 0.50939 0.04419 0.81133
N'10+ N 0.71484 0.08196 0.71877
O11+ O 1.25832 0.09251 0.51372
O12+ O -0.14095 0.34414 0.91744
H*13+ H 1.11639 0.05783 0.58149

#END

data_01600_-1.59853E+02
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 23.293
_cell_length_b 10.238
_cell_length_c 3.804
_cell_angle_alpha 90.00
_cell_angle_beta 86.16
_cell_angle_gamma 90.00
_cell_volume 905.117
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.59279 -0.27605 0.47853
N2 N 0.57105 -0.15700 0.42999
H*3 H 0.59461 -0.08640 0.30307

H*4 H 0.53043 -0.13417 0.51881
N5 N 0.64669 -0.30354 0.35814
H*6 H 0.66396 -0.39285 0.39197
H*7 H 0.67174 -0.23582 0.22981
N8 N 0.56062 -0.36760 0.64746
H*9 H 0.51980 -0.34889 0.74055
H*10 H 0.57620 -0.45816 0.68697
N'1+ N 0.21776 0.58869 -0.04740
N2+ N 0.21690 0.39930 -0.25706
N'3+ N 0.24910 0.50615 -0.24122
N'4+ N 0.16609 0.53719 0.06177
C5+ C 0.16544 0.41649 -0.07151
C6+ C 0.12416 0.31180 -0.05556
N7+ N 0.07059 0.30328 0.10798
N'8+ N 0.05035 0.18151 0.03677
N'9+ N 0.09064 0.12076 -0.16153
N'10+ N 0.13626 0.19749 -0.22288
O11+ O 0.23647 0.29184 -0.44082
O12+ O 0.04236 0.38767 0.29382
H*13+ H 0.20299 0.22841 -0.40377

#END

S31. Optimized crystal structure coordinates for 5 polymorphs of **4e** (ionic form).

data_04701_-1.61864E+02
_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 5.700
_cell_length_b 9.067
_cell_length_c 19.778
_cell_angle_alpha 90.00
_cell_angle_beta 104.25
_cell_angle_gamma 90.00
_cell_volume 990.714
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.20254 0.42744 -0.32142
N2 N -0.24870 0.47578 -0.38740
H*3 H -0.13800 0.54843 -0.40287
H*4 H -0.39586 0.44081 -0.42355
N5 N -0.00440 0.47678 -0.27480

H*6 H 0.10753 0.54975 -0.29001
N7 N -0.34834 0.33184 -0.30110
H*8 H -0.49854 0.29236 -0.33453
H*9 H -0.30498 0.29883 -0.25055
N10 N 0.04287 0.42588 -0.20596
H*11 H 0.20455 0.37197 -0.19314
H*12 H 0.04366 0.51171 -0.17267
N'1+ N -0.33878 0.31468 0.33052
N2+ N -0.39023 0.18704 0.41414
N'3+ N -0.49068 0.22239 0.34809
N'4+ N -0.14274 0.33944 0.38388
C5+ C -0.17511 0.25822 0.43723
C6+ C -0.03693 0.23485 0.50774
N7+ N 0.17936 0.29101 0.54337
N'8+ N 0.22664 0.23171 0.60884
N'9+ N 0.04452 0.14387 0.61152
N'10+ N -0.11952 0.14322 0.55069
O11+ O -0.50132 0.09144 0.44963
O12+ O 0.31909 0.38096 0.52315
H*13+ H -0.38299 0.08708 0.49740

#END

data_08970_-1.60452E+02
_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 19.345
_cell_length_b 13.257
_cell_length_c 3.814
_cell_angle_alpha 90.00
_cell_angle_beta 74.37
_cell_angle_gamma 90.00
_cell_volume 941.956
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.18551 -0.54092 -0.07043
N2 N -0.11708 -0.55722 -0.25600
H*3 H -0.10248 -0.61970 -0.40987
H*4 H -0.07812 -0.50735 -0.24706
N5 N -0.23584 -0.60928 -0.08960

H*6 H -0.22153 -0.67219 -0.24366
N7 N -0.20467 -0.45868 0.13198
H*8 H -0.16847 -0.40574 0.15310
H*9 H -0.25719 -0.45005 0.26690
N10 N -0.30723 -0.59184 0.10483
H*11 H -0.33892 -0.58726 -0.06893
H*12 H -0.32492 -0.64788 0.29002
N'1+ N 0.67928 -0.31048 -0.48670
N2+ N 0.59369 -0.38394 -0.11994
N'3+ N 0.66227 -0.39462 -0.30314
N'4+ N 0.62309 -0.24590 -0.42543
C5+ C 0.56848 -0.29255 -0.19179
C6+ C 0.49505 -0.26609 -0.01957
N7+ N 0.45695 -0.18139 -0.04312
N'8+ N 0.38932 -0.19627 0.17796
N'9+ N 0.38782 -0.28651 0.32593
N'10+ N 0.45147 -0.33117 0.21123
O11+ O 0.55796 -0.45860 0.10315
O12+ O 0.47678 -0.10163 -0.22793
H*13+ H 0.50805 -0.42863 0.20115

#END

data_08834_-1.60439E+02
_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 4.326
_cell_length_b 11.788
_cell_length_c 10.327
_cell_angle_alpha 104.34
_cell_angle_beta 71.02
_cell_angle_gamma 78.68
_cell_volume 459.923
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.90256 0.31827 0.62093
N2 N 0.69799 0.36325 0.76264
H*3 H 0.53570 0.31974 0.80786
H*4 H 0.70049 0.44209 0.82829
N5 N 0.89143 0.21288 0.53712
H*6 H 0.72898 0.16873 0.58187
N7 N 1.11605 0.37559 0.56152

H*8 H 1.13167 0.45478 0.62082
H*9 H 1.26526 0.33758 0.45373
N10 N 1.10571 0.16635 0.38916
H*11 H 1.26868 0.08177 0.36450
H*12 H 0.96320 0.16158 0.32766
N'1+ N 0.38614 0.08692 -0.31704
N2+ N 0.00351 0.09025 -0.12762
N'3+ N 0.17086 0.02804 -0.26907
N'4+ N 0.36080 0.18568 -0.20944
C5+ C 0.11712 0.18800 -0.08862
C6+ C -0.03195 0.26747 0.06059
N7+ N 0.03277 0.36948 0.12749
N'8+ N -0.18311 0.40906 0.27073
N'9+ N -0.36791 0.33296 0.28726
N'10+ N -0.28220 0.24547 0.16116
O11+ O -0.24427 0.05398 -0.04202
O12+ O 0.24703 0.42241 0.07428
H*13+ H -0.32162 0.11826 0.05762

#END

data_01965_-1.60237E+02
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z
_cell_length_a 18.467
_cell_length_b 4.161
_cell_length_c 26.352
_cell_angle_alpha 90.00
_cell_angle_beta 67.80
_cell_angle_gamma 90.00
_cell_volume 1874.81
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.10154 0.33655 0.58893
N2 N 0.04889 0.43739 0.56875
H*3 H 0.00659 0.59612 0.58937

H*4 H 0.05005 0.35721 0.53227
N5 N 0.09796 0.44926 0.63772
H*6 H 0.05562 0.60874 0.65864
N7 N 0.15718 0.12766 0.56176
H*8 H 0.16175 0.03781 0.52508
H*9 H 0.19555 0.05928 0.57889
N10 N 0.15312 0.34306 0.65859
H*11 H 0.18499 0.53203 0.66342
H*12 H 0.12595 0.22836 0.69503
N'1+ N 0.04315 0.13475 0.29637
N2+ N 0.13672 -0.15264 0.29586
N'3+ N 0.09730 -0.06139 0.26525
N'4+ N 0.04692 0.17159 0.34635
C5+ C 0.10651 -0.01133 0.34612
C6+ C 0.14104 -0.07897 0.38560
N7+ N 0.12269 0.02779 0.43774
N'8+ N 0.17455 -0.11299 0.45659
N'9+ N 0.22166 -0.29585 0.41691
N'10+ N 0.20283 -0.28064 0.37300
O11+ O 0.19827 -0.36053 0.27603
O12+ O 0.06894 0.21978 0.46584
H*13+ H 0.21562 -0.38257 0.30821

#END

data_05831_-1.60111E+02
_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 8.738
_cell_length_b 12.573
_cell_length_c 9.470
_cell_angle_alpha 90.00
_cell_angle_beta 66.75
_cell_angle_gamma 90.00
_cell_volume 955.912
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.37657 0.57602 -0.29254
N2 N 0.31008 0.49544 -0.34179
H*3 H 0.28262 0.50294 -0.43543

H*4 H 0.28554 0.42482 -0.28647
N5 N 0.40738 0.66890 -0.36955
H*6 H 0.38009 0.67695 -0.46369
N7 N 0.41266 0.56607 -0.16930
H*8 H 0.39135 0.49770 -0.10860
H*9 H 0.46282 0.62954 -0.13697
N10 N 0.47684 0.75278 -0.31756
H*11 H 0.58916 0.77376 -0.40000
H*12 H 0.39825 0.81638 -0.28867
N'1+ N 0.09914 0.85827 0.06111
N2+ N 0.06638 0.69330 0.05553
N'3+ N 0.04790 0.78431 -0.00760
N'4+ N 0.15018 0.81676 0.16710
C5+ C 0.12942 0.71164 0.16376
C6+ C 0.15887 0.62311 0.24596
N7+ N 0.21979 0.61918 0.35761
N'8+ N 0.22166 0.51440 0.39515
N'9+ N 0.16388 0.45884 0.30858
N'10+ N 0.12439 0.52272 0.21621
O11+ O 0.02441 0.59840 0.01044
O12+ O 0.26773 0.69454 0.41988
H*13+ H 0.05213 0.54531 0.07796

#END

S32. Optimized crystal structure coordinates for 5 polymorphs of **4f** (ionic form).

data_00918_-1.53067E+02
_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 11.998
_cell_length_b 7.238
_cell_length_c 23.094
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 2005.52
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y

```
_atom_site_fract_z
C1 C 0.24619 0.43780 0.39636
N2 N 0.25394 0.39762 0.45280
H*3 H 0.18220 0.39422 0.47620
N4 N 0.14506 0.47157 0.37326
H*5 H 0.13836 0.50213 0.33054
N6 N 0.33747 0.44423 0.36355
H*7 H 0.41177 0.41787 0.38277
H*8 H 0.33401 0.47416 0.32090
N9 N 0.05092 0.46363 0.40901
N10 N 0.35932 0.36264 0.47658
H*11 H 0.36162 0.23243 0.49324
H*12 H 0.01191 0.58851 0.40995
H*13 H -0.00252 0.36423 0.39480
H*14 H 0.37602 0.45620 0.50835
N'1+ N -0.47622 0.65657 0.27576
N2+ N -0.30198 0.64006 0.27061
N'3+ N -0.39519 0.59892 0.24224
N'4+ N -0.43709 0.73392 0.32510
C5+ C -0.32607 0.72356 0.32192
C6+ C -0.23629 0.77936 0.35932
N7+ N -0.23705 0.86380 0.41190
N'8+ N -0.12818 0.88450 0.42800
N'9+ N -0.06578 0.81467 0.38634
N'10+ N -0.12910 0.74932 0.34376
O11+ O -0.19990 0.59879 0.24790
O12+ O -0.31927 0.91666 0.44242
H*13+ H -0.14687 0.64608 0.27892

#END

data_10208_-1.52779E+02
_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                 7.396
_cell_length_b                 11.768
_cell_length_c                 12.174
_cell_angle_alpha               90.00
_cell_angle_beta                83.39
_cell_angle_gamma                 90.00
_cell_volume                   1052.53
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.53286 0.74583 0.31033
N2 N 0.53638 0.74037 0.20026
H*3 H 0.55559 0.81407 0.15692
N4 N 0.55462 0.84735 0.35837
H*5 H 0.55215 0.85233 0.44171
N6 N 0.50813 0.65194 0.37140
H*7 H 0.49236 0.57746 0.33174
H*8 H 0.50490 0.65365 0.45450
N9 N 0.58030 0.94427 0.29167
N10 N 0.51369 0.63458 0.15078
H*11 H 0.62586 0.61567 0.09732
H*12 H 0.47824 1.00115 0.31205
H*13 H 0.70300 0.98050 0.29992
H*14 H 0.40162 0.63628 0.10942
N'1+ N 0.77502 0.46267 0.06900
N2+ N 0.77716 0.28479 0.07939
N'3+ N 0.74407 0.37061 0.01348
N'4+ N 0.82732 0.43788 0.16922
C5+ C 0.82879 0.32457 0.17604
C6+ C 0.87100 0.24494 0.25905
N7+ N 0.92492 0.26149 0.36089
N'8+ N 0.94608 0.15614 0.40484
N'9+ N 0.90598 0.08049 0.33136
N'10+ N 0.85959 0.13179 0.24142
O11+ O 0.75820 0.17466 0.04730
O12+ O 0.95273 0.35386 0.41043
H*13+ H 0.79230 0.13031 0.11364

#END

data_01067_-1.52756E+02
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P b c a'
_symmetry_Int_Tables_number      61
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,z
3 x,1/2-y,1/2+z
4 1/2-x,-y,1/2+z
5 -x,-y,-z
6 1/2+x,1/2-y,-z
7 -x,1/2+y,1/2-z
8 1/2+x,y,1/2-z
_cell_length_a                 7.952
_cell_length_b                 13.328
_cell_length_c                 20.760
_cell_angle_alpha               90.00
```

```
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
_cell_volume                   2200.23
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25126 0.50659 -0.14192
N2 N 0.23026 0.45487 -0.08722
H*3 H 0.12638 0.41079 -0.08346
N4 N 0.13548 0.49817 -0.18902
H*5 H 0.15031 0.53706 -0.23063
N6 N 0.38509 0.56558 -0.14954
H*7 H 0.46893 0.56961 -0.11284
H*8 H 0.40399 0.60538 -0.19027
N9 N -0.00359 0.43549 -0.17937
N10 N 0.35107 0.46392 -0.03841
H*11 H 0.40318 0.39565 -0.02907
H*12 H -0.11206 0.47595 -0.18151
H*13 H -0.00526 0.37983 -0.21295
H*14 H 0.29663 0.49154 0.00229
N'1+ N 0.03362 0.75221 0.00862
N2+ N 0.19725 0.65931 0.06079
N'3+ N 0.10127 0.66251 0.00836
N'4+ N 0.08406 0.80678 0.06010
C5+ C 0.18835 0.74774 0.09342
C6+ C 0.28352 0.75972 0.15185
N7+ N 0.29706 0.83863 0.19301
N'8+ N 0.40454 0.80945 0.24082
N'9+ N 0.45234 0.71670 0.22814
N'10+ N 0.38082 0.68406 0.17418
O11+ O 0.28777 0.57547 0.07584
O12+ O 0.22746 0.92442 0.19051
H*13+ H 0.34640 0.59589 0.11738

#END

data_02102_-1.52405E+02
_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                 9.048
_cell_length_b                 11.480
_cell_length_c                 5.916
_cell_angle_alpha                99.01
```

```
_cell_angle_beta                61.41
_cell_angle_gamma               83.39
_cell_volume                   519.961
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.27629 0.24900 0.93358
N2 N 0.16589 0.24732 0.84354
H*3 H 0.12844 0.16860 0.81672
N4 N 0.33235 0.14772 0.98415
H*5 H 0.41600 0.14813 1.05241
N6 N 0.32985 0.34966 0.97250
H*7 H 0.28431 0.42367 0.93181
H*8 H 0.41300 0.35342 1.04019
N9 N 0.27340 0.04357 0.94099
N10 N 0.10806 0.35289 0.79132
H*11 H -0.02261 0.37975 0.90726
H*12 H 0.37422 -0.02460 0.80212
H*13 H 0.20859 0.01782 1.11372
H*14 H 0.14263 0.33743 0.59639
N'1+ N 0.17331 -0.09276 0.33324
N2+ N 0.12366 -0.24965 0.47037
N'3+ N 0.08080 -0.17446 0.35110
N'4+ N 0.27477 -0.11381 0.43850
C5+ C 0.24336 -0.21374 0.52603
C6+ C 0.30711 -0.28332 0.65575
N7+ N 0.42453 -0.26788 0.73267
N'8+ N 0.43659 -0.36047 0.84684
N'9+ N 0.33001 -0.42784 0.83723
N'10+ N 0.24893 -0.38331 0.72184
O11+ O 0.05066 -0.34709 0.52166
O12+ O 0.51058 -0.18595 0.70937
H*13+ H 0.10823 -0.38568 0.61146

#END

data_03448_-1.52164E+02
_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                  7.327
_cell_length_b                  11.759
```

_cell_length_c 12.205
_cell_angle_alpha 90.00
_cell_angle_beta 98.84
_cell_angle_gamma 90.00
_cell_volume 1039.07
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.68252 0.74001 0.81254
N2 N 0.62848 0.73707 0.70269
H*3 H 0.62380 0.81196 0.66073
N4 N 0.72780 0.84067 0.86219
H*5 H 0.76890 0.84374 0.94537
N6 N 0.69129 0.64447 0.87182
H*7 H 0.65594 0.57071 0.83099
H*8 H 0.73155 0.64426 0.95471
N9 N 0.71699 0.93938 0.79733
N10 N 0.58157 0.63216 0.65153
H*11 H 0.66614 0.61553 0.59461
H*12 H 0.62458 0.99486 0.82193
H*13 H 0.84353 0.97661 0.80290
H*14 H 0.44770 0.63373 0.61360
N'1+ N -0.18725 0.46386 0.56500
N2+ N -0.18413 0.28604 0.57849
N'3+ N -0.24466 0.37113 0.51075
N'4+ N -0.09108 0.44020 0.66621
C5+ C -0.08890 0.32693 0.67500
C6+ C -0.01155 0.24823 0.75984
N7+ N 0.08781 0.26595 0.86196
N'8+ N 0.12629 0.16107 0.90795
N'9+ N 0.05212 0.08456 0.83537
N'10+ N -0.03305 0.13485 0.74405
O11+ O -0.21953 0.17552 0.54811
O12+ O 0.13943 0.35891 0.91019
H*13+ H -0.15696 0.13191 0.61559

#END

S33. Optimized crystal structure coordinates for 5 polymorphs of **4g** (ionic form).

data_01845_-1.49461E+02
_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                 7.502
_cell_length_b                 11.950
_cell_length_c                 12.469
_cell_angle_alpha               90.00
_cell_angle_beta                98.42
_cell_angle_gamma                 90.00
_cell_volume                   1105.78
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.46555 0.24731 -0.30939
N2 N 0.41565 0.25423 -0.41690
H*3 H 0.41414 0.18231 -0.46057
N4 N 0.46986 0.33966 -0.24801
H*5 H 0.43433 0.41328 -0.28607
N6 N 0.51114 0.14805 -0.26325
H*7 H 0.54818 0.14634 -0.18152
N8 N 0.52249 0.33020 -0.13583
N9 N 0.36864 0.35896 -0.46315
H*10 H 0.23886 0.35742 -0.50109
H*11 H 0.63424 0.37760 -0.11243
H*12 H 0.42069 0.35607 -0.09596
H*13 H 0.45242 0.37895 -0.51756
N14 N 0.50552 0.05277 -0.32919
H*15 H 0.63032 0.01767 -0.32288
H*16 H 0.41677 -0.00385 -0.30642
N'1+ N 0.24314 0.47747 0.08275
N2+ N 0.26751 0.30284 0.07634
N'3+ N 0.29374 0.39642 0.02307
N'4+ N 0.18491 0.43799 0.17328
C5+ C 0.20031 0.32672 0.16938
C6+ C 0.16233 0.23654 0.23903
N7+ N 0.09592 0.23702 0.33479
N'8+ N 0.08677 0.12781 0.36597
N'9+ N 0.14573 0.06548 0.29115
N'10+ N 0.19295 0.12917 0.21252
O11+ O 0.30663 0.20063 0.03671
O12+ O 0.04899 0.31929 0.38896
H*13+ H 0.27293 0.14732 0.09412

#END

data_08909_-1.49265E+02
_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                3.929
_cell_length_b                14.735
_cell_length_c                20.090
_cell_angle_alpha             90.00
_cell_angle_beta              112.24
_cell_angle_gamma             90.00
_cell_volume                  1076.56
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.63014 0.47260 -0.17732
N2 N 0.61910 0.55747 -0.15417
H*3 H 0.63112 0.56545 -0.10306
N4 N 0.61517 0.45828 -0.24427
H*5 H 0.59554 0.51355 -0.27580
N6 N 0.65615 0.40205 -0.13352
H*7 H 0.66376 0.33880 -0.15310
N8 N 0.62719 0.36894 -0.26718
N9 N 0.59187 0.63004 -0.20099
H*10 H 0.81404 0.67158 -0.17968
H*11 H 0.39360 0.35479 -0.31043
H*12 H 0.85018 0.36055 -0.28071
H*13 H 0.35746 0.66582 -0.20940
N14 N 0.67136 0.41883 -0.06379
H*15 H 0.45449 0.38855 -0.05671
H*16 H 0.91107 0.39431 -0.02699
N'1+ N 0.08615 0.16855 -0.17568
N2+ N 0.47413 0.10116 -0.08762
N'3+ N 0.28265 0.09410 -0.15795
N'4+ N 0.14719 0.22336 -0.11823
C5+ C 0.39436 0.18055 -0.06204
C6+ C 0.57355 0.20131 0.01322
N7+ N 0.54472 0.27440 0.05205
N'8+ N 0.77715 0.25904 0.12148
N'9+ N 0.93666 0.17976 0.12331
N'10+ N 0.81863 0.14269 0.05815
O11+ O 0.71160 0.03440 -0.05072
O12+ O 0.34712 0.34510 0.03144
H*13+ H 0.81284 0.05903 0.00040

#END

data_03414_-1.48975E+02
_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                   11.051
_cell_length_b                   9.374
_cell_length_c                   8.151
_cell_angle_alpha                 78.90
_cell_angle_beta                  84.27
_cell_angle_gamma                    132.17
_cell_volume                     582.849
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.19986 -0.17533 0.16016
N2 N -0.12324 -0.09486 0.27826
H*3 H -0.11280 0.01631 0.29822
N4 N -0.21695 -0.32241 0.12883
H*5 H -0.17012 -0.36868 0.19731
N6 N -0.25939 -0.10872 0.07340
H*7 H -0.31666 -0.17362 -0.01505
N8 N -0.29752 -0.40402 0.00477
N9 N -0.06211 -0.16712 0.36719
H*10 H -0.12219 -0.22868 0.49932
H*11 H -0.21465 -0.37876 -0.09456
H*12 H -0.40407 -0.55787 0.06358
H*13 H 0.06723 -0.04958 0.34118
N14 N -0.23995 0.04515 0.10852
H*15 H -0.16804 0.17101 -0.00336
H*16 H -0.35745 -0.00810 0.15478
N'1+ N 0.42833 1.16047 0.20888
N2+ N 0.39538 0.91752 0.34652
N'3+ N 0.49811 1.08994 0.20668
N'4+ N 0.28288 1.03705 0.34718
C5+ C 0.26161 0.88212 0.43510
C6+ C 0.13511 0.70233 0.59120
N7+ N -0.00843 0.63172 0.70238
N'8+ N -0.08184 0.45358 0.82947
N'9+ N 0.01523 0.42087 0.79407
N'10+ N 0.14872 0.56977 0.64953
O11+ O 0.42991 0.80204 0.38527
O12+ O -0.06966 0.70807 0.69716
H*13+ H 0.33078 0.68366 0.49648

#END

data_02563_-1.48738E+02
```

```
_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                  8.006
_cell_length_b                  11.219
_cell_length_c                  8.769
_cell_angle_alpha                51.68
_cell_angle_beta                 89.78
_cell_angle_gamma                   73.79
_cell_volume                    578.205
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.36119 0.30657 0.66719
N2 N -0.23718 0.36797 0.57523
H*3 H -0.22961 0.39201 0.44348
N4 N -0.37683 0.27267 0.84134
H*5 H -0.29215 0.29525 0.89870
N6 N -0.46957 0.27907 0.58500
H*7 H -0.56181 0.23244 0.65940
N8 N -0.50751 0.20858 0.93447
N9 N -0.12554 0.39559 0.66421
H*10 H -0.14159 0.51560 0.57170
H*11 H -0.44895 0.09741 1.07130
H*12 H -0.59473 0.28454 0.94944
H*13 H 0.00419 0.32847 0.69355
N14 N -0.45052 0.31554 0.40289
H*15 H -0.42013 0.21313 0.41950
H*16 H -0.56592 0.40027 0.29765
N'1+ N -0.27502 0.55622 0.02713
N2+ N -0.12903 0.33132 0.10651
N'3+ N -0.26680 0.46790 -0.02490
N'4+ N -0.14544 0.47934 0.18924
C5+ C -0.05223 0.33599 0.24010
C6+ C 0.09977 0.19920 0.39546
N7+ N 0.19989 0.17272 0.54529
N'8+ N 0.32814 0.02211 0.65009
N'9+ N 0.30408 -0.03762 0.56474
N'10+ N 0.16583 0.06732 0.40889
O11+ O -0.08126 0.20986 0.09674
O12+ O 0.18483 0.26418 0.58807
H*13+ H 0.02564 0.12439 0.21403

#END
```

```
data_00539_-1.48664E+02
_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                 4.017
_cell_length_b                 15.797
_cell_length_c                 17.389
_cell_angle_alpha               90.00
_cell_angle_beta                79.53
_cell_angle_gamma                 90.00
_cell_volume                   1085.07
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.89574 0.51365 -0.32451
N2 N 0.84155 0.43413 -0.34621
H*3 H 0.75373 0.42596 -0.39696
N4 N 1.01147 0.52796 -0.25807
H*5 H 1.05497 0.47684 -0.22579
N6 N 0.83420 0.57885 -0.36926
H*7 H 0.87852 0.63815 -0.35077
N8 N 1.06605 0.61166 -0.23669
N9 N 0.90784 0.36708 -0.29842
H*10 H 1.08817 0.32838 -0.32871
H*11 H 0.91795 0.62510 -0.18411
H*12 H 1.31414 0.62004 -0.23308
H*13 H 0.69198 0.33345 -0.27974
N14 N 0.71333 0.56221 -0.43842
H*15 H 0.48301 0.59000 -0.43623
H*16 H 0.87920 0.58493 -0.48519
N'1+ N 0.34226 0.18732 0.32272
N2+ N 0.04231 0.10937 0.40525
N'3+ N 0.26620 0.10778 0.33874
N'4+ N 0.17202 0.24003 0.37752
C5+ C -0.01930 0.19051 0.43017
C6+ C -0.25546 0.20606 0.50146
N7+ N -0.36123 0.27948 0.53885
N'8+ N -0.58800 0.25765 0.60429
N'9+ N -0.61429 0.17436 0.60524
N'10+ N -0.41473 0.14087 0.54333
O11+ O -0.09328 0.03632 0.43946
```

O12+ O -0.27690 0.35532 0.52007
H*13+ H -0.25097 0.05792 0.48798

#END

S34. Optimized crystal structure coordinates for 5 polymorphs of **5a** (ionic form).

data_09227_-1.86160E+02
_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 7.876
_cell_length_b 9.485
_cell_length_c 9.888
_cell_angle_alpha 90.00
_cell_angle_beta 100.59
_cell_angle_gamma 90.00
_cell_volume 726.09
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.51503 0.46968 0.76053
H*2 H 0.51855 0.38708 0.69382
H*3 H 0.62686 0.47068 0.83293
H*4 H 0.50392 0.56294 0.70669
H*5 H 0.41080 0.45802 0.80869
N'1+ N 0.77516 0.42672 -0.00756
N'2+ N 0.90848 0.24341 0.11073
N3+ N 0.85869 0.30217 -0.01339
N'4+ N 0.77060 0.44950 0.12458
C5+ C 0.85083 0.33890 0.19328
C6+ C 0.87357 0.32316 0.34145
N'7+ N 0.81608 0.41854 0.42505
N8+ N 0.86682 0.35779 0.54439
N'9+ N 0.94852 0.23678 0.54537
N'10+ N 0.95437 0.21220 0.41428
O11+ O 0.88580 0.24848 -0.12468
O12+ O 0.83510 0.41920 0.66287
H*13+ H 0.88591 0.35242 0.73341

#END

data_04886_-1.85826E+02
_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                   12.719
_cell_length_b                   7.877
_cell_length_c                   9.821
_cell_angle_alpha                  90.00
_cell_angle_beta                 49.22
_cell_angle_gamma                  90.00
_cell_volume                     745.064
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.52394 -0.50331 0.23572
H*2 H 0.54524 -0.60970 0.16082
H*3 H 0.50532 -0.40246 0.18762
H*4 H 0.43780 -0.52501 0.36786
H*5 H 0.60740 -0.47607 0.22658
N'1+ N 0.23675 0.92481 0.24673
N'2+ N 0.41578 0.79621 0.19929
N3+ N 0.35584 0.83434 0.13080
N'4+ N 0.21884 0.94606 0.39521
C5+ C 0.32678 0.86837 0.36399
C6+ C 0.34623 0.86229 0.49393
N'7+ N 0.25738 0.93440 0.65955
N8+ N 0.31908 0.89466 0.72164
N'9+ N 0.43498 0.80700 0.61546
N'10+ N 0.45464 0.78449 0.46641
O11+ O 0.40396 0.79143 -0.02481
O12+ O 0.26378 0.94342 0.89106
H*13+ H 0.32981 0.89755 0.90042

#END

data_00120_-1.85533E+02
_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 8.007
_cell_length_b 9.548
_cell_length_c 13.921
_cell_angle_alpha 90.00
_cell_angle_beta 43.52
_cell_angle_gamma 90.00
_cell_volume 732.866
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.28311 0.49043 0.24017
H*2 H 0.33807 0.56946 0.17209
H*3 H 0.35538 0.39698 0.18714
H*4 H 0.34196 0.51122 0.28421
H*5 H 0.09703 0.48406 0.31724
N'1+ N 0.48544 -0.23977 0.44771
N'2+ N 0.22527 -0.41854 0.57533
N3+ N 0.39107 -0.35890 0.44899
N'4+ N 0.37739 -0.22152 0.57738
C5+ C 0.22297 -0.32932 0.65172
C6+ C 0.06870 -0.34840 0.79946
N'7+ N 0.06530 -0.25931 0.87691
N8+ N -0.09753 -0.32073 0.99863
N'9+ N -0.19556 -0.43666 1.00646
N'10+ N -0.08996 -0.45665 0.87793
O11+ O 0.45439 -0.40732 0.34173
O12+ O -0.16153 -0.26512 1.11257
H*13+ H -0.28254 -0.33099 1.18625

#END

data_06734_-1.85436E+02
_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 9.845
_cell_length_b 7.851
_cell_length_c 9.451
_cell_angle_alpha 90.00
_cell_angle_beta 81.21

```
_cell_angle_gamma               90.00
_cell_volume                   721.917
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.75973 0.46893 0.50967
H*2 H 0.81972 0.57653 0.49520
H*3 H 0.82168 0.36291 0.50192
H*4 H 0.70065 0.47240 0.60919
H*5 H 0.69686 0.46388 0.43238
N'1+ N 0.03951 0.71775 0.07068
N'2+ N -0.08876 0.57536 0.24929
N3+ N 0.03799 0.62487 0.19220
N'4+ N -0.09044 0.72886 0.04821
C5+ C -0.16517 0.64306 0.15598
C6+ C -0.31330 0.62464 0.17105
N'7+ N -0.39076 0.69221 0.07784
N8+ N -0.51289 0.64142 0.13688
N'9+ N -0.52097 0.55088 0.25493
N'10+ N -0.39217 0.53839 0.27915
O11+ O 0.14542 0.58972 0.24479
O12+ O -0.62700 0.68202 0.07674
H*13+ H -0.70099 0.62892 0.14176

#END

data_09137_-1.85279E+02
_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                 6.448
_cell_length_b                 12.736
_cell_length_c                 17.862
_cell_angle_alpha               90.00
_cell_angle_beta                32.83
_cell_angle_gamma               90.00
_cell_volume                   795.255
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

_atom_site_fract_z
N1 N 0.35833 -0.04364 -0.31472
H*2 H 0.25125 -0.02871 -0.33476
H*3 H 0.33817 -0.12261 -0.29743
H*4 H 0.64024 -0.02094 -0.39795
H*5 H 0.20366 -0.00230 -0.22874
N'1+ N 0.78567 0.19556 -0.32594
N'2+ N 0.91844 0.07476 -0.27840
N3+ N 0.88793 0.09465 -0.34253
N'4+ N 0.74865 0.24265 -0.24855
C5+ C 0.82913 0.16917 -0.22139
C6+ C 0.82123 0.18895 -0.13902
N'7+ N 0.73187 0.28351 -0.08143
N8+ N 0.76466 0.26098 -0.02022
N'9+ N 0.86308 0.16439 -0.03257
N'10+ N 0.90142 0.11610 -0.10955
O11+ O 0.94722 0.02739 -0.41139
O12+ O 0.69808 0.33598 0.05354
H*13+ H 0.74261 0.29797 0.08642

#END

S35. Optimized crystal structure coordinates for 5 polymorphs of **5b** (ionic form).

data_02777_-1.90129E+02
_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 9.677
_cell_length_b 13.834
_cell_length_c 6.068
_cell_angle_alpha 90.00
_cell_angle_beta 74.34
_cell_angle_gamma 90.00
_cell_volume 782.18
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.30068 0.42823 0.26051
H*2 H 0.31258 0.35446 0.27045
H*3 H 0.32517 0.46022 0.39912
H*4 H 0.36852 0.45272 0.10879
O5 O 0.15564 0.44128 0.26650
H*6 H 0.13972 0.51071 0.25740

N'1+ N 0.16719 0.17902 0.16856
N'2+ N 0.24117 0.07514 0.39741
N3+ N 0.16983 0.08585 0.23805
N'4+ N 0.23911 0.23042 0.28662
C5+ C 0.28227 0.16704 0.42203
C6+ C 0.36487 0.19431 0.57937
N'7+ N 0.40656 0.28640 0.60511
N8+ N 0.47535 0.27298 0.76091
N'9+ N 0.48159 0.18421 0.83505
N'10+ N 0.41033 0.13176 0.71912
O11+ O 0.11088 0.01716 0.15947
O12+ O 0.53791 0.34923 0.84199
H*13+ H 0.58002 0.31858 0.95273

#END

data_03453_-1.89243E+02
_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 20.278
_cell_length_b 6.004
_cell_length_c 28.963
_cell_angle_alpha 90.00
_cell_angle_beta 24.72
_cell_angle_gamma 90.00
_cell_volume 1474.61
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.42131 0.41880 -0.11585
H*2 H 0.39608 0.37134 -0.06641
H*3 H 0.53014 0.49604 -0.18557
H*4 H 0.42154 0.27903 -0.13679
O5 O 0.29929 0.56653 -0.05017
H*6 H 0.31886 0.61579 -0.09424
N'1+ N 0.18007 -0.28022 0.14483
N'2+ N 0.15092 -0.59620 0.20396

N3+ N 0.18216 -0.50643 0.14276
N'4+ N 0.14641 -0.22132 0.20945
C5+ C 0.12950 -0.41233 0.24381
C6+ C 0.09194 -0.42101 0.31653
N'7+ N 0.07025 -0.23721 0.35690
N8+ N 0.04024 -0.33121 0.41577
N'9+ N 0.04058 -0.55010 0.41701
N'10+ N 0.07399 -0.61210 0.35292
O11+ O 0.21068 -0.61849 0.08855
O12+ O 0.00985 -0.20422 0.47346
H*13+ H -0.00774 -0.31566 0.50844

#END

data_03286_-1.88858E+02
_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 9.188
_cell_length_b 11.118
_cell_length_c 7.482
_cell_angle_alpha 90.00
_cell_angle_beta 97.30
_cell_angle_gamma 90.00
_cell_volume 758.108
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.38455 0.00126 0.80026
H*2 H 0.36286 -0.07363 0.87365
H*3 H 0.49038 -0.00479 0.76814
H*4 H 0.30971 0.00488 0.68503
O5 O 0.36814 0.09872 0.91573
H*6 H 0.38789 0.17197 0.85090
N'1+ N 0.33070 -0.03899 0.29042
N'2+ N 0.18167 -0.19959 0.28018
N3+ N 0.27897 -0.13816 0.19703
N'4+ N 0.26487 -0.03597 0.43894
C5+ C 0.17649 -0.13256 0.43008
C6+ C 0.08441 -0.16227 0.56759
N'7+ N 0.07857 -0.09546 0.71847
N8+ N -0.01686 -0.15793 0.79543

N'9+ N -0.07094 -0.25505 0.71136
N'10+ N -0.00650 -0.25963 0.56263
O11+ O 0.31916 -0.16836 0.04768
O12+ O -0.05777 -0.12238 0.95741
H*13+ H -0.12782 -0.18405 0.98119

#END

data_06191_-1.88381E+02
_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 8.510
_cell_length_b 11.635
_cell_length_c 7.966
_cell_angle_alpha 90.00
_cell_angle_beta 91.75
_cell_angle_gamma 90.00
_cell_volume 788.376
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.32528 -0.04691 0.22131
H*2 H 0.32719 -0.11708 0.30033
H*3 H 0.22178 -0.00229 0.23678
H*4 H 0.42137 0.00438 0.25044
O5 O 0.33332 -0.09395 0.05923
H*6 H 0.33180 -0.02988 -0.02001
N'1+ N 0.25288 0.68646 0.25529
N'2+ N 0.27094 0.56038 0.46844
N3+ N 0.21422 0.58048 0.31252
N'4+ N 0.33741 0.73674 0.37803
C5+ C 0.34672 0.66004 0.50391
C6+ C 0.42982 0.68175 0.66247
N'7+ N 0.50619 0.78155 0.69907
N8+ N 0.55953 0.75866 0.85115
N'9+ N 0.52589 0.65727 0.91350
N'10+ N 0.44148 0.60573 0.79274
O11+ O 0.13327 0.50915 0.22664
O12+ O 0.64691 0.83817 0.94042
H*13+ H 0.66970 0.79871 1.04595

```
#END

data_10656_-1.88143E+02
_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                 6.247
_cell_length_b                 14.766
_cell_length_c                 17.404
_cell_angle_alpha               90.00
_cell_angle_beta                149.52
_cell_angle_gamma               90.00
_cell_volume                   814.32
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.33764 0.46882 -0.22472
H*2 H 0.25386 0.52862 -0.27709
H*3 H 0.63458 0.45014 -0.15153
H*4 H 0.33532 0.47844 -0.16665
O5 O 0.02767 0.40647 -0.34390
H*6 H 0.09580 0.34849 -0.29885
N'1+ N 0.99376 0.17982 -0.38896
N'2+ N 0.95640 0.08337 -0.30100
N3+ N 0.96473 0.09210 -0.37501
N'4+ N 1.00463 0.22961 -0.32186
C5+ C 0.98197 0.17072 -0.27021
C6+ C 0.98460 0.19797 -0.18931
N'7+ N 1.01019 0.28551 -0.15794
N8+ N 1.00120 0.27418 -0.08619
N'9+ N 0.97327 0.19066 -0.06911
N'10+ N 0.96204 0.13990 -0.13541
O11+ O 0.94760 0.02628 -0.42681
O12+ O 1.02042 0.34719 -0.03163
H*13+ H 1.00797 0.31911 0.01499

#END
```

S36. Optimized crystal structure coordinates for 5 polymorphs of **5c** (ionic form).

```
data_07798_-1.84057E+02
_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                 8.453
_cell_length_b                 13.247
_cell_length_c                 6.916
_cell_angle_alpha               90.00
_cell_angle_beta                81.48
_cell_angle_gamma                 90.00
_cell_volume                   765.886
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.82241 0.43340 -0.22578
H*2 H 0.85503 0.35859 -0.22598
H*3 H 0.79229 0.45414 -0.08169
N4 N 0.68067 0.44159 -0.31945
H*5 H 0.64802 0.51589 -0.31669
H*6 H 0.71112 0.41979 -0.46180
H*7 H 0.92000 0.47544 -0.28703
N'1+ N 0.72692 0.16701 -0.32201
N'2+ N 0.78555 0.06697 -0.08029
N3+ N 0.71755 0.07294 -0.24295
N'4+ N 0.80345 0.22392 -0.20694
C5+ C 0.83730 0.16274 -0.06374
C6+ C 0.92112 0.19594 0.09339
N'7+ N 0.97346 0.29195 0.11105
N8+ N 1.03864 0.28306 0.27035
N'9+ N 1.03333 0.19367 0.35372
N'10+ N 0.95731 0.13576 0.24091
O11+ O 0.65141 -0.00057 -0.31637
O12+ O 1.10925 0.36446 0.34561
H*13+ H 1.14627 0.33632 0.46078

#END

data_09452_-1.83798E+02
_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 6.417
_cell_length_b 13.056
_cell_length_c 17.193
_cell_angle_alpha 90.00
_cell_angle_beta 32.87
_cell_angle_gamma 90.00
_cell_volume 781.774
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.84625 0.57059 0.71467
H*2 H 0.90591 0.64333 0.67643
H*3 H 0.72100 0.53218 0.70828
N4 N 0.56640 0.57845 0.86441
H*5 H 0.50553 0.50587 0.90197
H*6 H 0.69150 0.61767 0.86994
H*7 H 1.10133 0.53470 0.64870
N'1+ N 0.22165 0.16238 0.22235
N'2+ N 0.35483 0.06167 0.28298
N3+ N 0.32504 0.06753 0.21478
N'4+ N 0.18311 0.21991 0.29789
C5+ C 0.26387 0.15832 0.33296
C6+ C 0.25463 0.19199 0.41624
N'7+ N 0.16360 0.28888 0.46681
N8+ N 0.19574 0.28007 0.53224
N'9+ N 0.29520 0.18996 0.52865
N'10+ N 0.33506 0.13141 0.45364
O11+ O 0.38591 -0.00671 0.14997
O12+ O 0.12745 0.36228 0.60138
H*13+ H 0.17186 0.33400 0.63899

#END

data_01860_-1.83206E+02
_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 8.853
_cell_length_b 12.793
_cell_length_c 7.375

```
_cell_angle_alpha                90.00
_cell_angle_beta                 86.99
_cell_angle_gamma                90.00
_cell_volume                    834.114
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.34743 0.55604 0.75124
H*2 H -0.35305 0.62376 0.67670
H*3 H -0.45395 0.52372 0.75594
N4 N -0.31188 0.58383 0.93450
H*5 H -0.30818 0.51631 1.00810
H*6 H -0.20671 0.61692 0.92841
H*7 H -0.27329 0.50516 0.68393
N'1+ N 0.25471 0.18735 0.26023
N'2+ N 0.29317 0.07661 0.48950
N3+ N 0.22964 0.09031 0.33036
N'4+ N 0.33714 0.23823 0.37764
C5+ C 0.35876 0.17074 0.51331
C6+ C 0.44403 0.19613 0.67012
N'7+ N 0.51023 0.29044 0.69504
N8+ N 0.57057 0.27400 0.85065
N'9+ N 0.55017 0.18141 0.92538
N'10+ N 0.46805 0.12941 0.81011
O11+ O 0.15422 0.02098 0.25250
O12+ O 0.65160 0.35107 0.93094
H*13+ H 0.68191 0.31767 1.04172

#END

data_07851_-1.83047E+02
_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                  6.765
_cell_length_b                  8.200
_cell_length_c                  8.581
_cell_angle_alpha                85.36
_cell_angle_beta                 67.50
_cell_angle_gamma                110.52
_cell_volume                    398.953
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.49893 0.31594 0.27734
H*2 H 0.53406 0.44870 0.23625
H*3 H 0.44768 0.29058 0.40939
N4 N 0.71564 0.29378 0.19480
H*5 H 0.67982 0.16213 0.23776
H*6 H 0.76669 0.32115 0.06363
H*7 H 0.36055 0.23658 0.25503
N'1+ N 0.36318 0.32867 -0.11210
N'2+ N 0.29433 0.04543 -0.13576
N3+ N 0.35920 0.21456 -0.21829
N'4+ N 0.29884 0.23043 0.04434
C5+ C 0.25863 0.06197 0.02727
C6+ C 0.18420 -0.08777 0.16951
N'7+ N 0.14796 -0.07229 0.33355
N8+ N 0.08536 -0.23899 0.40949
N'9+ N 0.07819 -0.35590 0.31327
N'10+ N 0.14192 -0.26033 0.15648
O11+ O 0.41149 0.26421 -0.37779
O12+ O 0.02993 -0.28778 0.58270
H*13+ H -0.00877 -0.41590 0.60276

#END

data_10570_-1.82682E+02
_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                 5.452
_cell_length_b                 15.327
_cell_length_c                 9.359
_cell_angle_alpha               90.00
_cell_angle_beta                84.05
_cell_angle_gamma                 90.00
_cell_volume                   777.851
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.78549 0.64206 0.64988
H*2 H 0.87115 0.58449 0.67168
```

H*3 H 0.67809 0.62908 0.56829
N4 N 0.97366 0.70412 0.59700
H*5 H 0.88697 0.76075 0.57410
H*6 H 1.08113 0.71590 0.67808
H*7 H 0.67218 0.66074 0.73998
N'1+ N 0.52291 0.38290 -0.43150
N'2+ N 0.71615 0.31032 -0.26737
N3+ N 0.54261 0.30701 -0.35858
N'4+ N 0.68900 0.43721 -0.38615
C5+ C 0.80212 0.39259 -0.28832
C6+ C 0.99739 0.42891 -0.21244
N'7+ N 1.08475 0.51144 -0.23284
N8+ N 1.25254 0.51210 -0.14257
N'9+ N 1.28028 0.44041 -0.06875
N'10+ N 1.11595 0.38536 -0.11255
O11+ O 0.41027 0.24074 -0.37585
O12+ O 1.39250 0.58517 -0.12676
H*13+ H 1.49842 0.56719 -0.05469

#END

S37. Optimized crystal structure coordinates for 5 polymorphs of **5d** (ionic form).

data_05658_-1.77982E+02
_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 7.123
_cell_length_b 17.271
_cell_length_c 7.196
_cell_angle_alpha 90.00
_cell_angle_beta 92.42
_cell_angle_gamma 90.00
_cell_volume 884.472
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.28627 -0.17179 0.65823
N2 N -0.45505 -0.17145 0.73290
H*3 H -0.52132 -0.22132 0.76331
H*4 H -0.52124 -0.12132 0.76110
N5 N -0.20194 -0.23902 0.62238
H*6 H -0.07443 -0.24059 0.56600
H*7 H -0.26326 -0.29021 0.65063

N8 N -0.20183 -0.10490 0.61941
H*9 H -0.26305 -0.05346 0.64538
H*10 H -0.07432 -0.10385 0.56297
N'1+ N 0.85828 0.39158 0.06932
N'2+ N 0.62217 0.32391 0.18781
N3+ N 0.78713 0.32044 0.10550
N'4+ N 0.73554 0.44287 0.13011
C5+ C 0.59585 0.40126 0.20022
C6+ C 0.43264 0.43575 0.28137
N'7+ N 0.40516 0.51334 0.29435
N8+ N 0.24391 0.51431 0.37483
N'9+ N 0.16790 0.44713 0.41340
N'10+ N 0.28844 0.39515 0.35372
O11+ O 0.86913 0.25800 0.06516
O12+ O 0.15926 0.58315 0.41644
H*13+ H 0.04482 0.56651 0.47372

#END

data_03697_-1.77228E+02
_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 7.268
_cell_length_b 17.267
_cell_length_c 16.262
_cell_angle_alpha 90.00
_cell_angle_beta 117.37
_cell_angle_gamma 90.00
_cell_volume 1812.37
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.75743 -0.07768 -0.14364
N2 N 0.75523 -0.01039 -0.10338
H*3 H 0.75891 0.04078 -0.13274
H*4 H 0.74981 -0.00875 -0.04241
N5 N 0.76464 -0.07811 -0.22434

H*6 H 0.76642 -0.12829 -0.25595
H*7 H 0.76851 -0.02826 -0.25608
N8 N 0.75243 -0.14454 -0.10320
H*9 H 0.74695 -0.14553 -0.04223
H*10 H 0.75397 -0.19602 -0.13243
N'1+ N 0.24462 0.64246 -0.42971
N'2+ N 0.25414 0.57477 -0.30992
N3+ N 0.25074 0.57131 -0.39289
N'4+ N 0.24403 0.69373 -0.36869
C5+ C 0.24976 0.65210 -0.29779
C6+ C 0.25114 0.68657 -0.21616
N'7+ N 0.24677 0.76415 -0.20345
N8+ N 0.25025 0.76511 -0.12232
N'9+ N 0.25622 0.69792 -0.08310
N'10+ N 0.25690 0.64595 -0.14301
O11+ O 0.25294 0.50889 -0.43325
O12+ O 0.24770 0.83393 -0.08071
H*13+ H 0.25127 0.81727 -0.02288

#END

data_08356_-1.77181E+02
_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 4.927
_cell_length_b 17.278
_cell_length_c 16.251
_cell_angle_alpha 90.00
_cell_angle_beta 138.71
_cell_angle_gamma 90.00
_cell_volume 912.882
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.54390 0.67331 0.34389
N2 N -0.53085 0.60655 0.38843
H*3 H -0.51460 0.55518 0.36259
H*4 H -0.53685 0.60554 0.44923
N5 N -0.53551 0.67292 0.26353
H*6 H -0.54508 0.72269 0.22874
H*7 H -0.51935 0.62284 0.23524

N8 N -0.56534 0.74046 0.37971
H*9 H -0.57202 0.74206 0.44034
H*10 H -0.57550 0.79155 0.34720
N'1+ N 0.47561 -0.10598 0.06524
N'2+ N 0.46624 -0.17398 0.18085
N3+ N 0.46577 -0.17719 0.09839
N'4+ N 0.48269 -0.05493 0.12820
C5+ C 0.47692 -0.09673 0.19654
C6+ C 0.48167 -0.06253 0.27915
N'7+ N 0.49239 0.01496 0.29543
N8+ N 0.49251 0.01567 0.37595
N'9+ N 0.48322 -0.05158 0.41166
N'10+ N 0.47605 -0.10333 0.34977
O11+ O 0.45715 -0.23944 0.05540
O12+ O 0.50202 0.08432 0.42048
H*13+ H 0.49971 0.06751 0.47704

#END

data_04781_-1.77030E+02
_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 3.904
_cell_length_b 16.129
_cell_length_c 14.730
_cell_angle_alpha 90.00
_cell_angle_beta 87.24
_cell_angle_gamma 90.00
_cell_volume 926.437
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.49019 -0.38448 0.67320
N2 N 0.34413 -0.42851 0.74157
H*3 H 0.35011 -0.49115 0.74133
H*4 H 0.22351 -0.40044 0.79547
N5 N 0.64811 -0.42329 0.60271
H*6 H 0.76012 -0.39122 0.55035
H*7 H 0.66005 -0.48583 0.59975
N8 N 0.47833 -0.30164 0.67532
H*9 H 0.36033 -0.27107 0.72793

H*10 H 0.58701 -0.26718 0.62438
N'1+ N 1.22262 0.90700 -0.09175
N'2+ N 1.26350 0.78562 -0.16616
N3+ N 1.35636 0.86555 -0.16552
N'4+ N 1.03702 0.85220 -0.04296
C5+ C 1.06498 0.78025 -0.08857
C6+ C 0.89882 0.70415 -0.05779
N'7+ N 0.69913 0.69823 0.02001
N8+ N 0.61415 0.61987 0.01693
N'9+ N 0.73592 0.57644 -0.05295
N'10+ N 0.92205 0.63009 -0.10250
O11+ O 1.54775 0.89945 -0.22662
O12+ O 0.40609 0.58529 0.08444
H*13+ H 0.38725 0.52802 0.06472

#END

data_00569_-1.76729E+02
_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 8.329
_cell_length_b 16.358
_cell_length_c 6.786
_cell_angle_alpha 90.00
_cell_angle_beta 82.67
_cell_angle_gamma 90.00
_cell_volume 917.008
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.34357 0.35905 0.67254
N2 N -0.47672 0.39954 0.74847
H*3 H -0.57678 0.36960 0.81025
H*4 H -0.48115 0.46127 0.74629
N5 N -0.34112 0.27733 0.67746
H*6 H -0.24179 0.24554 0.62094
H*7 H -0.43853 0.24500 0.73785
N8 N -0.21287 0.40027 0.59169
H*9 H -0.21214 0.46201 0.58643
H*10 H -0.11103 0.37088 0.53348
N'1+ N 0.21741 0.42584 0.39924

N'2+ N 0.35515 0.30855 0.33976
N3+ N 0.36236 0.39034 0.33635
N'4+ N 0.11279 0.36514 0.44492
C5+ C 0.19750 0.29574 0.40834
C6+ C 0.12708 0.21492 0.43922
N'7+ N -0.03107 0.20153 0.50801
N8+ N -0.03318 0.12158 0.50920
N'9+ N 0.10369 0.08368 0.44984
N'10+ N 0.20972 0.14329 0.40355
O11+ O 0.48967 0.43080 0.28087
O12+ O -0.17353 0.07981 0.57036
H*13+ H -0.13971 0.02302 0.55585

#END

S38. Optimized crystal structure coordinates for 5 polymorphs of **5e** (ionic form).

data_04050_-1.75725E+02
_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 9.108
_cell_length_b 6.752
_cell_length_c 10.500
_cell_angle_alpha 67.99
_cell_angle_beta 122.73
_cell_angle_gamma 114.10
_cell_volume 485.777
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.57560 0.72968 -0.34365
N2 N 0.56827 0.68432 -0.21126
H*3 H 0.68187 0.69638 -0.10940
H*4 H 0.44863 0.63669 -0.20969
N5 N 0.73782 0.79266 -0.34077
H*6 H 0.85244 0.80510 -0.23884
N7 N 0.42602 0.71375 -0.47764
H*8 H 0.30199 0.66707 -0.48443
H*9 H 0.43922 0.74999 -0.57441
N10 N 0.74462 0.83982 -0.47943
H*11 H 0.81448 1.00017 -0.50092
H*12 H 0.80343 0.73549 -0.47458
N'1+ N 0.24987 0.52986 -0.18421
N'2+ N -0.04751 0.50715 -0.32248
N3+ N 0.11286 0.58763 -0.32357

N'4+ N 0.17603 0.40798 -0.08966
C5+ C -0.00137 0.39656 -0.17450
C6+ C -0.13103 0.27741 -0.11366
N'7+ N -0.08581 0.16596 0.03475
N8+ N -0.24483 0.09038 0.03115
N'9+ N -0.38296 0.14087 -0.10074
N'10+ N -0.31195 0.26261 -0.19670
O11+ O 0.13587 0.70492 -0.44096
O12+ O -0.26450 -0.03628 0.16077
H*13+ H -0.39353 -0.06785 0.12486

#END

data_04274_-1.74894E+02
_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 16.673
_cell_length_b 6.861
_cell_length_c 19.367
_cell_angle_alpha 90.00
_cell_angle_beta 117.20
_cell_angle_gamma 90.00
_cell_volume 1970.46
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.53475 0.70059 0.07409
N2 N 0.53141 0.65375 0.13989
H*3 H 0.58818 0.62950 0.18976
H*4 H 0.47187 0.64136 0.14141
N5 N 0.61549 0.71564 0.07450
H*6 H 0.67277 0.69147 0.12441
N7 N 0.45999 0.73246 0.00848
H*8 H 0.39825 0.72255 0.00588
H*9 H 0.46634 0.76748 -0.03967
N10 N 0.61855 0.76461 0.00560
H*11 H 0.65273 0.89198 0.01233

H*12 H 0.64837 0.65577 -0.01020
N'1+ N 0.37516 0.61352 0.15979
N'2+ N 0.22483 0.60421 0.08714
N3+ N 0.30520 0.59919 0.08726
N'4+ N 0.33903 0.62831 0.20828
C5+ C 0.24932 0.62245 0.16373
C6+ C 0.18490 0.63446 0.19458
N'7+ N 0.20893 0.65278 0.27139
N8+ N 0.12920 0.65714 0.26885
N'9+ N 0.05874 0.64383 0.20017
N'10+ N 0.09344 0.62894 0.15094
O11+ O 0.31564 0.58292 0.02675
O12+ O 0.12054 0.67494 0.33569
H*13+ H 0.05553 0.67409 0.31660

#END

data_02140_-1.74663E+02
_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 10.016
_cell_length_b 6.529
_cell_length_c 16.592
_cell_angle_alpha 30.09
_cell_angle_beta 82.25
_cell_angle_gamma 73.28
_cell_volume 506.073
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.19668 0.46832 0.34982
N2 N -0.30569 0.42466 0.41608
H*3 H -0.39291 0.39642 0.40531
H*4 H -0.30362 0.41877 0.47878
N5 N -0.20361 0.47466 0.26716
H*6 H -0.29092 0.44644 0.25590
N7 N -0.08195 0.50545 0.36406
H*8 H -0.07286 0.50211 0.42509
H*9 H -0.00249 0.53772 0.31156
N10 N -0.08942 0.52035 0.19822
H*11 H -0.04475 0.25562 0.24881
H*12 H -0.12397 0.79629 0.07313
N'1+ N -0.32656 0.42624 0.58617

N'2+ N -0.19426 0.33879 0.71786
N3+ N -0.19387 0.34532 0.63489
N'4+ N -0.41592 0.47375 0.63924
C5+ C -0.33476 0.42031 0.71742
C6+ C -0.39193 0.44723 0.79398
N'7+ N -0.53284 0.52895 0.79409
N8+ N -0.52879 0.51996 0.87562
N'9+ N -0.40317 0.44299 0.92609
N'10+ N -0.31247 0.39460 0.87427
O11+ O -0.08265 0.28329 0.60446
O12+ O -0.65162 0.58870 0.90626
H*13+ H -0.61705 0.56369 0.96720

#END

data_01263_-1.73659E+02
_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 3.929
_cell_length_b 21.722
_cell_length_c 11.515
_cell_angle_alpha 90.00
_cell_angle_beta 106.23
_cell_angle_gamma 90.00
_cell_volume 943.591
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.87488 0.59133 0.77707
N2 N 0.76046 0.55906 0.67436
H*3 H 0.62405 0.51938 0.67133
H*4 H 0.80762 0.57356 0.59696
N5 N 0.80650 0.57042 0.87831
H*6 H 0.66961 0.53060 0.87588
N7 N 1.05438 0.64354 0.78096
H*8 H 1.11074 0.66069 0.70695
H*9 H 1.13484 0.66616 0.86103
N10 N 0.92669 0.60433 0.98532
H*11 H 0.71791 0.61817 1.01506
H*12 H 1.09800 0.57865 1.04990
N'1+ N 0.35798 0.04687 0.14743

N'2+ N 0.15911 0.12535 0.23739
N3+ N 0.34216 0.07253 0.25339
N'4+ N 0.17947 0.08425 0.05987
C5+ C 0.06318 0.13075 0.11554
C6+ C -0.14490 0.18178 0.05148
N'7+ N -0.24231 0.18754 -0.07082
N8+ N -0.41913 0.23927 -0.08269
N'9+ N -0.44371 0.26633 0.01680
N'10+ N -0.26699 0.22968 0.10529
O11+ O 0.48589 0.04867 0.35566
O12+ O -0.57133 0.26373 -0.19507
H*13+ H -0.68176 0.30113 -0.17657

#END

data_05378_-1.73436E+02
_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 8.171
_cell_length_b 16.463
_cell_length_c 18.403
_cell_angle_alpha 90.00
_cell_angle_beta 157.24
_cell_angle_gamma 90.00
_cell_volume 957.723
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.94408 -0.07112 0.21076
N2 N -1.00782 -0.07686 0.25646
H*3 H -1.02630 -0.02689 0.28061
H*4 H -1.03922 -0.13147 0.26804
N5 N -0.90383 0.00283 0.19676
H*6 H -0.92208 0.05327 0.22084
N7 N -0.91981 -0.13692 0.17901
H*8 H -0.94844 -0.19338 0.18816
H*9 H -0.87121 -0.12914 0.14488
N10 N -0.83730 0.00845 0.14898
H*11 H -1.07818 0.03973 0.02651
H*12 H -0.55565 0.03618 0.25391
N'1+ N -0.09873 0.44039 -0.19003

N'2+ N -0.09113 0.30425 -0.17969
N3+ N -0.08325 0.36896 -0.22055
N'4+ N -0.11724 0.42142 -0.12735
C5+ C -0.11233 0.33993 -0.12228
C6+ C -0.12819 0.29451 -0.06128
N'7+ N -0.14951 0.32987 -0.00344
N8+ N -0.15658 0.26516 0.03490
N'9+ N -0.14233 0.19413 0.00814
N'10+ N -0.12374 0.21180 -0.05448
O11+ O -0.06357 0.36475 -0.28110
O12+ O -0.17804 0.27212 0.10030
H*13+ H -0.17855 0.21582 0.11602

#END

S39. Optimized crystal structure coordinates for 5 polymorphs of **5f** (ionic form).

data_08293_-1.67180E+02
_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 8.448
_cell_length_b 17.184
_cell_length_c 7.542
_cell_angle_alpha 90.00
_cell_angle_beta 79.14
_cell_angle_gamma 90.00
_cell_volume 1075.27
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.18881 0.03017 -0.11707
N2 N 0.09138 0.08075 -0.17863
H*3 H 0.06350 0.07016 -0.30176
N4 N 0.24506 -0.03176 -0.21945
H*5 H 0.31894 -0.07039 -0.17395
N6 N 0.22946 0.04109 0.04345
H*7 H 0.18432 0.08848 0.11582
H*8 H 0.30268 0.00389 0.09308
N9 N 0.19988 -0.04142 -0.38744
N10 N 0.03328 0.14504 -0.07157
H*11 H -0.08937 0.14347 -0.04122
H*12 H 0.29889 -0.04052 -0.48804
H*13 H 0.13891 -0.09237 -0.39037

H*14 H 0.07025 0.19520 -0.13866
N'1+ N 0.39659 -0.07430 0.19284
N'2+ N 0.42752 -0.20346 0.21602
N3+ N 0.37403 -0.14561 0.12389
N'4+ N 0.46699 -0.08628 0.33425
C5+ C 0.48429 -0.16369 0.34560
C6+ C 0.55673 -0.20112 0.48321
N'7+ N 0.61401 -0.16162 0.61377
N8+ N 0.66478 -0.21972 0.70020
N'9+ N 0.64622 -0.29026 0.63974
N'10+ N 0.57607 -0.27954 0.49845
O11+ O 0.30930 -0.15559 -0.01273
O12+ O 0.73435 -0.20662 0.84780
H*13+ H 0.75949 -0.25891 0.88321

#END

data_07343_-1.66678E+02
_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 8.639
_cell_length_b 10.937
_cell_length_c 11.337
_cell_angle_alpha 90.00
_cell_angle_beta 88.49
_cell_angle_gamma 90.00
_cell_volume 1070.8
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.67718 0.14336 -0.13179
N2 N 0.77571 0.09507 -0.21214
H*3 H 0.84805 0.02799 -0.18504
N4 N 0.67802 0.10161 -0.01996
H*5 H 0.60379 0.13763 0.04153
N6 N 0.57966 0.23158 -0.16227
H*7 H 0.58309 0.26014 -0.24739
H*8 H 0.50421 0.26956 -0.10350
N9 N 0.78205 0.00882 0.00897
N10 N 0.77431 0.13886 -0.32828
H*11 H 0.74816 0.06956 -0.38435

H*12 H 0.85549 0.03862 0.07159
H*13 H 0.72352 -0.06654 0.03828
H*14 H 0.87982 0.17448 -0.35111
N'1+ N 0.37752 0.35336 -0.00978
N'2+ N 0.28244 0.36430 0.17617
N3+ N 0.37537 0.30360 0.10004
N'4+ N 0.28295 0.44944 -0.00475
C5+ C 0.22752 0.45426 0.10694
C6+ C 0.11936 0.54678 0.14935
N'7+ N 0.06367 0.63739 0.08042
N8+ N -0.02591 0.69420 0.15740
N'9+ N -0.03281 0.65026 0.26538
N'10+ N 0.06091 0.55422 0.26215
O11+ O 0.45326 0.20997 0.12654
O12+ O -0.10861 0.79544 0.12541
H*13+ H -0.16313 0.81763 0.19841

#END

data_07648_-1.66649E+02
_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 4.660
_cell_length_b 18.270
_cell_length_c 17.355
_cell_angle_alpha 90.00
_cell_angle_beta 45.53
_cell_angle_gamma 90.00
_cell_volume 1054.42
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.79007 0.42166 0.22985
N2 N 0.67323 0.48761 0.22675
H*3 H 0.55181 0.52260 0.28874
N4 N 0.74249 0.40466 0.31382
H*5 H 0.83011 0.35483 0.31687
N6 N 0.95125 0.37354 0.15079
H*7 H 0.98126 0.38868 0.08924
H*8 H 1.04186 0.32346 0.15112
N9 N 0.57203 0.45655 0.39548

N10 N 0.72345 0.50497 0.13923
H*11 H 0.90724 0.54926 0.09930
H*12 H 0.31321 0.43676 0.46756
H*13 H 0.77008 0.47009 0.40063
H*14 H 0.45143 0.51601 0.16608
N'1+ N 1.00534 0.19075 0.13680
N'2+ N 0.98219 0.11347 0.24168
N3+ N 0.99199 0.11991 0.16298
N'4+ N 1.00417 0.23158 0.20056
C5+ C 0.99028 0.18439 0.26244
C6+ C 0.98449 0.20711 0.34362
N'7+ N 0.99254 0.27819 0.36495
N8+ N 0.98266 0.26963 0.44162
N'9+ N 0.96951 0.20222 0.47053
N'10+ N 0.97045 0.16060 0.40774
O11+ O 0.98923 0.06623 0.11738
O12+ O 0.98606 0.32915 0.48917
H*13+ H 0.97688 0.30683 0.54172

#END

data_10127_-1.66582E+02
_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 4.831
_cell_length_b 17.951
_cell_length_c 17.421
_cell_angle_alpha 90.00
_cell_angle_beta 136.05
_cell_angle_gamma 90.00
_cell_volume 1048.52
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.26986 0.58186 0.77221
N2 N 0.14517 0.51595 0.77409
H*3 H 0.01901 0.48001 0.71090
N4 N 0.22356 0.59757 0.68783
H*5 H 0.31710 0.64736 0.68569
N6 N 0.43751 0.63120 0.85285
H*7 H 0.46626 0.61700 0.91466

H*8 H 0.53409 0.68127 0.85347
N9 N 0.04616 0.54443 0.60449
N10 N 0.19411 0.49993 0.86204
H*11 H 0.37014 0.45412 0.90357
H*12 H -0.20811 0.56525 0.53007
H*13 H 0.23970 0.52868 0.60114
H*14 H -0.07663 0.49061 0.83266
N'1+ N 0.49497 0.19228 0.14796
N'2+ N 0.49711 0.11220 0.24741
N3+ N 0.49239 0.11984 0.17000
N'4+ N 0.50157 0.23296 0.21317
C5+ C 0.50274 0.18408 0.27176
C6+ C 0.50939 0.20608 0.35321
N'7+ N 0.51507 0.27812 0.37814
N8+ N 0.51953 0.26834 0.45344
N'9+ N 0.51734 0.19935 0.47836
N'10+ N 0.51074 0.15787 0.41406
O11+ O 0.48619 0.06585 0.12203
O12+ O 0.52621 0.32825 0.50364
H*13+ H 0.52828 0.30482 0.55437

#END

data_05557_-1.65667E+02
_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 7.829
_cell_length_b 18.008
_cell_length_c 7.432
_cell_angle_alpha 90.00
_cell_angle_beta 87.90
_cell_angle_gamma 90.00
_cell_volume 1047.09
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.21976 0.02794 0.24866
N2 N 0.28100 0.09363 0.19191
H*3 H 0.19512 0.13327 0.15896
N4 N 0.04929 0.01726 0.25957
H*5 H 0.00171 -0.03232 0.30242

N6 N 0.32634 -0.02610 0.29369
H*7 H 0.45356 -0.01559 0.28337
H*8 H 0.28363 -0.07613 0.33687
N9 N -0.05894 0.07527 0.21117
N10 N 0.45836 0.10441 0.18084
H*11 H 0.49112 0.14694 0.26303
H*12 H -0.13072 0.05963 0.10614
H*13 H -0.13608 0.09045 0.31816
H*14 H 0.49648 0.11620 0.05150
N'1+ N -0.30949 0.70177 -0.22764
N'2+ N -0.10592 0.61960 -0.15980
N3+ N -0.26027 0.62942 -0.22809
N'4+ N -0.18302 0.74011 -0.15679
C5+ C -0.06297 0.69002 -0.11730
C6+ C 0.09715 0.70941 -0.03697
N'7+ N 0.14125 0.77997 0.00610
N8+ N 0.29154 0.76809 0.07185
N'9+ N 0.34623 0.69908 0.07500
N'10+ N 0.22165 0.65991 0.00476
O11+ O -0.35148 0.57739 -0.28701
O12+ O 0.38675 0.82591 0.13449
H*13+ H 0.48927 0.80124 0.17402

#END

S40. Optimized crystal structure coordinates for 5 polymorphs of **5g** (ionic form).

data_07030_-1.63016E+02
_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 3.839
_cell_length_b 18.316
_cell_length_c 15.466
_cell_angle_alpha 90.00
_cell_angle_beta 79.15
_cell_angle_gamma 90.00
_cell_volume 1068.05
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.02667 -0.84836 0.65965
N2 N -0.06476 -0.92053 0.67246
H*3 H -0.02997 -0.94078 0.73144

N4 N -0.06969 -0.81885 0.58303
H*5 H -0.13105 -0.85304 0.53634
N6 N 0.05444 -0.80570 0.72346
H*7 H 0.08101 -0.75126 0.71117
N8 N -0.02844 -0.74327 0.57128
N9 N -0.14959 -0.96394 0.60473
H*10 H -0.38506 -0.98979 0.62587
H*11 H 0.17167 -0.73264 0.51954
H*12 H -0.25815 -0.72082 0.55983
H*13 H 0.04475 -1.00160 0.58558
N14 N 0.09802 -0.83787 0.80294
H*15 H 0.34829 -0.82857 0.81340
H*16 H -0.08152 -0.81675 0.85368
N'1+ N 0.31209 -0.13714 -0.42747
N'2+ N 0.46044 -0.19012 -0.30856
N3+ N 0.40584 -0.19981 -0.39081
N'4+ N 0.30566 -0.08511 -0.36708
C5+ C 0.39495 -0.11790 -0.29670
C6+ C 0.41897 -0.07974 -0.21584
N'7+ N 0.35366 -0.00725 -0.20341
N8+ N 0.40938 0.00000 -0.12298
N'9+ N 0.50100 -0.05884 -0.08395
N'10+ N 0.50887 -0.11142 -0.14324
O11+ O 0.43735 -0.26050 -0.43069
O12+ O 0.37261 0.06668 -0.08187
H*13+ H 0.42890 0.05587 -0.02451

#END

data_09348_-1.63015E+02
_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 3.878
_cell_length_b 19.228
_cell_length_c 14.723
_cell_angle_alpha 90.00
_cell_angle_beta 86.99
_cell_angle_gamma 90.00
_cell_volume 1096.32
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y

```
_atom_site_fract_z
C1 C 0.62435 0.65100 -0.17035
N2 N 0.74051 0.69130 -0.23969
H*3 H 0.83716 0.73877 -0.22438
N4 N 0.49429 0.58791 -0.18679
H*5 H 0.48830 0.57255 -0.25276
N6 N 0.63825 0.67379 -0.08456
H*7 H 0.54759 0.64168 -0.03391
N8 N 0.37457 0.54679 -0.11314
N9 N 0.72312 0.66628 -0.32873
H*10 H 0.96468 0.66365 -0.35922
H*11 H 0.11898 0.53617 -0.11817
H*12 H 0.51061 0.50151 -0.11230
H*13 H 0.57306 0.69831 -0.36509
N14 N 0.77535 0.73993 -0.06918
H*15 H 0.59357 0.77050 -0.03660
H*16 H 0.98520 0.73585 -0.03073
N'1+ N 1.34287 -0.12968 -0.41570
N'2+ N 1.03778 -0.18092 -0.30038
N3+ N 1.21076 -0.18999 -0.38065
N'4+ N 1.25271 -0.07989 -0.35626
C5+ C 1.07097 -0.11160 -0.28802
C6+ C 0.92440 -0.07518 -0.20878
N'7+ N 0.95654 -0.00560 -0.19587
N8+ N 0.78554 0.00112 -0.11739
N'9+ N 0.65139 -0.05551 -0.07999
N'10+ N 0.73866 -0.10584 -0.13836
O11+ O 1.24868 -0.24816 -0.42019
O12+ O 0.74985 0.06504 -0.07659
H*13+ H 0.61477 0.05449 -0.02079

#END

data_10573_-1.63012E+02
_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                 3.840
_cell_length_b                 18.314
_cell_length_c                 15.465
_cell_angle_alpha               90.00
_cell_angle_beta                79.15
_cell_angle_gamma                 90.00
_cell_volume                   1068.15
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.47310 0.15161 -0.34031
N2 N 0.43011 0.18114 -0.41693
H*3 H 0.36882 0.14695 -0.46364
N4 N 0.55413 0.19427 -0.27648
H*5 H 0.58066 0.24871 -0.28875
N6 N 0.43506 0.07943 -0.32752
H*7 H 0.46982 0.05917 -0.26854
N8 N 0.59767 0.16207 -0.19700
N9 N 0.47131 0.25673 -0.42866
H*10 H 0.24162 0.27917 -0.44012
H*11 H 0.84790 0.17139 -0.18653
H*12 H 0.41810 0.18318 -0.14625
H*13 H 0.67141 0.26738 -0.48039
N14 N 0.35032 0.03603 -0.39527
H*15 H 0.54468 -0.00163 -0.41443
H*16 H 0.11489 0.01017 -0.37415
N'1+ N 0.81201 -0.13721 -0.42747
N'2+ N 0.96060 -0.19016 -0.30856
N3+ N 0.90593 -0.19987 -0.39080
N'4+ N 0.80553 -0.08517 -0.36708
C5+ C 0.89496 -0.11794 -0.29670
C6+ C 0.91898 -0.07976 -0.21584
N'7+ N 0.85352 -0.00728 -0.20341
N8+ N 0.90930 -0.00001 -0.12298
N'9+ N 1.00109 -0.05884 -0.08396
N'10+ N 1.00902 -0.11143 -0.14324
O11+ O 0.93754 -0.26057 -0.43068
O12+ O 0.87243 0.06668 -0.08188
H*13+ H 0.92880 0.05588 -0.02451

#END

data_01213_-1.63003E+02
_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                 3.879
_cell_length_b                 19.232
_cell_length_c                 16.275
_cell_angle_alpha               90.00
```

```
_cell_angle_beta                64.55
_cell_angle_gamma               90.00
_cell_volume                    1096.31
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.78354 0.34897 0.17044
N2 N 0.62076 0.41206 0.18692
H*3 H 0.48288 0.42742 0.25292
N4 N 0.96895 0.32618 0.08461
H*5 H 0.97969 0.35830 0.03396
N6 N 0.76090 0.30867 0.23979
H*7 H 0.88805 0.26119 0.22444
N8 N 1.13665 0.26005 0.06919
N9 N 0.64847 0.45318 0.11326
H*10 H 0.78631 0.49844 0.11239
H*11 H 1.01994 0.22950 0.03663
H*12 H 1.42341 0.26410 0.03067
H*13 H 0.38284 0.46383 0.11835
N14 N 0.56551 0.33368 0.32887
H*15 H 0.34264 0.30167 0.36528
H*16 H 0.74611 0.33628 0.35932
N'1+ N -0.01128 -0.12969 0.58428
N'2+ N 0.06314 -0.18091 0.69961
N3+ N 0.05077 -0.18998 0.61933
N'4+ N -0.04009 -0.07991 0.64373
C5+ C 0.00517 -0.11160 0.71197
C6+ C -0.00683 -0.07518 0.79122
N'7+ N -0.06489 -0.00561 0.80414
N8+ N -0.05090 0.00111 0.88263
N'9+ N 0.00849 -0.05549 0.92002
N'10+ N 0.03805 -0.10582 0.86164
O11+ O 0.09201 -0.24814 0.57978
O12+ O -0.09690 0.06503 0.92343
H*13+ H -0.07344 0.05448 0.97923

#END

data_08448_-1.62469E+02
_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                 3.862
_cell_length_b                 16.144
_cell_length_c                 17.630
_cell_angle_alpha               90.00
_cell_angle_beta                86.24
_cell_angle_gamma                 90.00
_cell_volume                   1096.83
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.07742 0.86332 -0.15625
N2 N 0.09684 0.84562 -0.08235
H*3 H 0.01312 0.78889 -0.06408
N4 N 0.18437 0.93726 -0.18331
H*5 H 0.27850 0.97819 -0.14597
N6 N -0.04895 0.80707 -0.20309
H*7 H -0.05936 0.82288 -0.25870
N8 N 0.16137 0.95425 -0.26077
N9 N 0.22992 0.90547 -0.03458
H*10 H 0.44472 0.88305 -0.01100
H*11 H 0.00426 1.00406 -0.26730
H*12 H 0.40186 0.96612 -0.28557
H*13 H 0.04713 0.92098 0.00727
N14 N -0.15903 0.73025 -0.17340
H*15 H -0.41552 0.72182 -0.18132
H*16 H -0.01792 0.68389 -0.19959
N'1+ N 0.45414 0.41251 0.36646
N'2+ N 0.54989 0.28574 0.31701
N3+ N 0.59574 0.36737 0.30722
N'4+ N 0.31184 0.35842 0.41628
C5+ C 0.37199 0.28321 0.38565
C6+ C 0.25765 0.20669 0.42246
N'7+ N 0.07894 0.20361 0.49136
N8+ N 0.03951 0.12349 0.49881
N'9+ N 0.17119 0.07647 0.44324
N'10+ N 0.31452 0.12937 0.39290
O11+ O 0.75339 0.39965 0.24932
O12+ O -0.13297 0.09076 0.56241
H*13+ H -0.12245 0.03153 0.55256

#END
```

S41. Optimized crystal structure coordinates for 5 polymorphs of **6a** (ionic form).

```
data_03276_-1.67276E+02
_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 4.893
_cell_length_b 10.036
_cell_length_c 16.169
_cell_angle_alpha 90.00
_cell_angle_beta 61.33
_cell_angle_gamma 90.00
_cell_volume 696.651
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.27498 0.13419 -0.16131
H*2 H 0.29553 0.18498 -0.10936
H*3 H 0.36946 0.04063 -0.16872
H*4 H 0.04358 0.12608 -0.14325
H*5 H 0.39134 0.18507 -0.22391
N'1+ N 0.10341 -0.10443 0.57812
N'2+ N 0.31346 -0.03247 0.66758
N3+ N 0.21642 -0.13837 0.63681
N'4+ N 0.12797 0.02806 0.57053
C5+ C 0.25342 0.06849 0.62433
C6+ C 0.30634 0.20970 0.62896
N7+ N 0.23008 0.29815 0.57982
N'8+ N 0.29735 0.42178 0.59384
N'9+ N 0.41450 0.40952 0.65135
N'10+ N 0.42362 0.28062 0.67444
O11+ O 0.22934 -0.25675 0.66018
O12+ O 0.10242 0.27306 0.52274
H*13+ H 0.07970 0.17206 0.52662

#END

data_06306_-1.66923E+02
_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 6.674
_cell_length_b 10.649
_cell_length_c 10.661

```
_cell_angle_alpha                90.00
_cell_angle_beta                 108.40
_cell_angle_gamma                90.00
_cell_volume                     718.956
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.30926 0.09557 0.86750
H*2 H -0.40204 0.06611 0.92259
H*3 H -0.16753 0.12803 0.92950
H*4 H -0.28261 0.02163 0.81285
H*5 H -0.38486 0.16651 0.80506
N'1+ N -1.02303 -0.04113 0.25660
N'2+ N -1.16545 0.14472 0.28521
N3+ N -1.18430 0.04059 0.20973
N'4+ N -0.89512 0.01179 0.36628
C5+ C -0.98315 0.12215 0.38118
C6+ C -0.87563 0.19991 0.49385
N7+ N -0.69045 0.16124 0.58165
N'8+ N -0.61886 0.24604 0.67701
N'9+ N -0.75932 0.33653 0.64807
N'10+ N -0.91933 0.31141 0.53617
O11+ O -1.33615 0.02115 0.10625
O12+ O -0.58216 0.05297 0.58025
H*13+ H -0.67537 0.00944 0.49726

#END

data_03673_-1.66921E+02
_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                   4.938
_cell_length_b                   19.837
_cell_length_c                   7.241
_cell_angle_alpha                90.00
_cell_angle_beta                 80.82
_cell_angle_gamma                90.00
_cell_volume                     700.208
loop_
_atom_site_label
_atom_site_type_symbol
```

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.02283 0.39054 -0.32424
H*2 H -0.18441 0.42332 -0.29069
H*3 H -0.09656 0.34239 -0.33315
H*4 H 0.08951 0.40409 -0.45071
H*5 H 0.10014 0.39236 -0.22241
N'1+ N 0.67799 0.22816 0.20795
N'2+ N 0.31296 0.28257 0.36851
N3+ N 0.43357 0.22245 0.32119
N'4+ N 0.71736 0.29426 0.18084
C5+ C 0.49766 0.32552 0.27767
C6+ C 0.48708 0.39848 0.27261
N7+ N 0.69535 0.43389 0.17197
N'8+ N 0.64497 0.49974 0.18618
N'9+ N 0.40674 0.50486 0.29510
N'10+ N 0.30359 0.44366 0.35089
O11+ O 0.32991 0.16667 0.37648
O12+ O 0.92954 0.40980 0.06748
H*13+ H 0.90738 0.35904 0.08459

#END

data_00141_-1.66921E+02
_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                 6.676
_cell_length_b                 10.648
_cell_length_c                 10.660
_cell_angle_alpha               90.00
_cell_angle_beta                71.59
_cell_angle_gamma                 90.00
_cell_volume                   718.995
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.69071 -0.09560 0.63250
H*2 H 0.59793 -0.06603 0.57747
H*3 H 0.61508 -0.16655 0.69493
H*4 H 0.83233 -0.12810 0.57042
```

H*5 H 0.71750 -0.02171 0.68717
N'1+ N 0.02297 -0.04118 0.75657
N'2+ N 0.16549 0.14463 0.78522
N3+ N 0.18429 0.04050 0.70973
N'4+ N -0.10492 0.01177 0.86624
C5+ C -0.01684 0.12211 0.88117
C6+ C -0.12432 0.19989 0.99386
N7+ N -0.30954 0.16128 1.08163
N'8+ N -0.38109 0.24609 1.17700
N'9+ N -0.24058 0.33654 1.14809
N'10+ N -0.08057 0.31138 1.03620
O11+ O 0.33613 0.02102 0.60625
O12+ O -0.41789 0.05304 1.08020
H*13+ H -0.32469 0.00948 0.99722

#END

data_01563_-1.66920E+02
_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 4.935
_cell_length_b 19.838
_cell_length_c 7.243
_cell_angle_alpha 90.00
_cell_angle_beta 80.80
_cell_angle_gamma 90.00
_cell_volume 699.972
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.02271 0.39054 0.32412
H*2 H -0.08966 0.40412 0.45056
H*3 H -0.10030 0.39240 0.22234
H*4 H 0.18456 0.42327 0.29054
H*5 H 0.09624 0.34237 0.33304
N'1+ N 0.32183 0.27182 0.29204
N'2+ N 0.68704 0.21741 0.13137
N3+ N 0.56637 0.27752 0.17872
N'4+ N 0.28245 0.20572 0.31916
C5+ C 0.50225 0.17446 0.22226
C6+ C 0.51284 0.10150 0.22731

N7+ N 0.30448 0.06609 0.32802
N'8+ N 0.35488 0.00025 0.31379
N'9+ N 0.59322 -0.00488 0.20480
N'10+ N 0.69641 0.05632 0.14898
O11+ O 0.67007 0.33330 0.12340
O12+ O 0.07017 0.09018 0.43258
H*13+ H 0.09235 0.14094 0.41546

#END

S42. Optimized crystal structure coordinates for 5 polymorphs of **6b** (ionic form).

data_02478_-1.72461E+02
_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 8.380
_cell_length_b 19.260
_cell_length_c 4.623
_cell_angle_alpha 90.00
_cell_angle_beta 83.64
_cell_angle_gamma 90.00
_cell_volume 741.554
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.52516 -0.37231 0.04558
H*2 H 0.60951 -0.39205 -0.11226
H*3 H 0.49542 -0.41025 0.20012
H*4 H 0.57286 -0.32933 0.13832
O5 O 0.39394 -0.35465 -0.10464
H*6 H 0.31072 -0.33561 0.03802
N'1+ N 0.33210 -0.02183 0.25138
N'2+ N 0.21240 0.04214 0.62318
N3+ N 0.21255 -0.01803 0.47236
N'4+ N 0.41230 0.03794 0.25906
C5+ C 0.33887 0.07506 0.48185
C6+ C 0.40215 0.14304 0.54002
N7+ N 0.53258 0.16810 0.37201
N'8+ N 0.57061 0.23097 0.46206
N'9+ N 0.46408 0.24457 0.68453
N'10+ N 0.35866 0.19172 0.73875
O11+ O 0.11195 -0.06585 0.53065
O12+ O 0.61950 0.13708 0.14066

H*13+ H 0.56167 0.09088 0.12734

#END

data_09213_-1.72428E+02
_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 4.746
_cell_length_b 10.285
_cell_length_c 15.198
_cell_angle_alpha 90.00
_cell_angle_beta 82.38
_cell_angle_gamma 90.00
_cell_volume 735.303
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.05890 0.42801 0.84179
H*2 H -0.00364 0.52361 0.83816
H*3 H -0.05387 0.37228 0.80197
H*4 H 0.27463 0.42184 0.82086
O5 O -0.00767 0.39518 0.93194
H*6 H 0.04863 0.30468 0.93831
N'1+ N 0.70616 -0.16678 0.10008
N'2+ N 0.31438 -0.09065 0.18491
N3+ N 0.47800 -0.19539 0.15996
N'4+ N 0.69006 -0.03907 0.08568
C5+ C 0.45546 0.00395 0.13684
C6+ C 0.38622 0.14097 0.13409
N7+ N 0.55586 0.22303 0.08083
N'8+ N 0.45449 0.34372 0.08828
N'9+ N 0.22345 0.33602 0.14586
N'10+ N 0.17483 0.21291 0.17542
O11+ O 0.42451 -0.30829 0.18926
O12+ O 0.79845 0.19463 0.02561
H*13+ H 0.81850 0.09713 0.03472

#END

data_01675_-1.71585E+02
_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                   5.076
_cell_length_b                   7.604
_cell_length_c                   9.762
_cell_angle_alpha                101.64
_cell_angle_beta                 84.09
_cell_angle_gamma                91.65
_cell_volume                     367.07
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.44867 0.21211 0.29820
H*2 H 0.30596 0.28042 0.37061
H*3 H 0.40131 0.21545 0.19836
H*4 H 0.63042 0.27256 0.31541
O5 O 0.43852 0.03645 0.32373
H*6 H 0.57166 -0.03323 0.25685
N'1+ N -0.30842 0.39272 0.62300
N'2+ N 0.06258 0.23095 0.60987
N3+ N -0.10541 0.30488 0.53893
N'4+ N -0.27088 0.37519 0.75297
C5+ C -0.04919 0.27855 0.74243
C6+ C 0.03848 0.23917 0.86956
N7+ N -0.10159 0.29917 0.99576
N'8+ N 0.01247 0.24849 1.09817
N'9+ N 0.22185 0.15769 1.03532
N'10+ N 0.24417 0.14919 0.89482
O11+ O -0.07681 0.29356 0.40796
O12+ O -0.32796 0.39770 1.02351
H*13+ H -0.36369 0.41416 0.92613

#END

data_00263_-1.71525E+02
_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 10.184
_cell_length_b 9.921
_cell_length_c 7.652
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 773.123
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.10577 0.45804 0.32198
H*2 H 0.14998 0.52581 0.23857
H*3 H 0.17505 0.42296 0.40946
H*4 H 0.02999 0.50598 0.38669
O5 O 0.05942 0.35479 0.21229
H*6 H 0.01655 0.28800 0.28669
N'1+ N 0.02467 0.19655 0.49710
N'2+ N -0.04968 0.08063 0.73088
N3+ N -0.07288 0.12035 0.56467
N'4+ N 0.11428 0.20662 0.62384
C5+ C 0.06785 0.13690 0.76142
C6+ C 0.14663 0.13113 0.91891
N7+ N 0.26438 0.19503 0.92583
N'8+ N 0.32026 0.17706 1.08127
N'9+ N 0.23729 0.10243 1.16969
N'10+ N 0.12947 0.07226 1.07408
O11+ O -0.17475 0.08984 0.48067
O12+ O 0.32435 0.26904 0.79869
H*13+ H 0.25854 0.26382 0.69872

#END

data_07236_-1.71496E+02
_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 4.912
_cell_length_b 19.116
_cell_length_c 7.431
_cell_angle_alpha 90.00
_cell_angle_beta 87.06

```
_cell_angle_gamma              90.00
_cell_volume                  696.836
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.61723 0.10064 -0.21758
H*2 H 0.55934 0.14793 -0.16106
H*3 H 0.47313 0.08543 -0.30619
H*4 H 0.80608 0.10638 -0.28367
O5 O 0.62690 0.05459 -0.07053
H*6 H 0.68136 0.00884 -0.11854
N'1+ N 0.29249 0.56655 0.11497
N'2+ N -0.08176 0.55634 0.30248
N3+ N 0.11535 0.52269 0.20256
N'4+ N 0.20740 0.63090 0.15958
C5+ C -0.01527 0.62345 0.27110
C6+ C -0.15055 0.68589 0.34084
N7+ N -0.05286 0.75011 0.29372
N'8+ N -0.20622 0.79997 0.37215
N'9+ N -0.39750 0.76661 0.46715
N'10+ N -0.36976 0.69643 0.45116
O11+ O 0.13324 0.45719 0.19165
O12+ O 0.16839 0.76617 0.18316
H*13+ H 0.23992 0.71803 0.14584

#END
```

S43. Optimized crystal structure coordinates for 5 polymorphs of **6c** (ionic form).

```
data_05481_-1.68263E+02
_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                 9.281
_cell_length_b                 9.965
_cell_length_c                 7.994
_cell_angle_alpha               90.00
_cell_angle_beta                84.26
_cell_angle_gamma              90.00
_cell_volume                  735.619
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.58386 0.39684 -0.26151
H*2 H 0.65252 0.38513 -0.36975
H*3 H 0.51332 0.31697 -0.25596
N4 N 0.50108 0.51857 -0.27733
H*5 H 0.43207 0.52867 -0.17022
H*6 H 0.57206 0.59722 -0.28466
H*7 H 0.64380 0.39210 -0.15955
N'1+ N 0.26358 0.45503 -0.01749
N'2+ N 0.13974 0.26354 0.04494
N3+ N 0.25204 0.32232 -0.04824
N'4+ N 0.15503 0.48335 0.09969
C5+ C 0.08300 0.36794 0.13472
C6+ C -0.04152 0.36999 0.25945
N7+ N -0.08343 0.48632 0.33825
N'8+ N -0.19935 0.46611 0.44732
N'9+ N -0.22870 0.33791 0.43575
N'10+ N -0.13397 0.27564 0.32153
O11+ O 0.33753 0.26036 -0.15316
O12+ O -0.02230 0.61033 0.31682
H*13+ H 0.06178 0.59294 0.22751

#END

data_05448_-1.67596E+02
_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                 8.134
_cell_length_b                 9.555
_cell_length_c                 11.728
_cell_angle_alpha               90.00
_cell_angle_beta                54.45
_cell_angle_gamma                 90.00
_cell_volume                   741.608
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.82513 0.47423 -0.27543
H*2 H 0.83370 0.56815 -0.23629
H*3 H 0.79004 0.49735 -0.34462
```

N4 N 0.65943 0.39467 -0.16064
H*5 H 0.65051 0.30230 -0.20062
H*6 H 0.69441 0.37350 -0.09167
H*7 H 0.96528 0.42676 -0.32970
N'1+ N -0.21287 0.92840 0.47097
N'2+ N -0.13755 0.73369 0.54101
N3+ N -0.15475 0.79291 0.44366
N'4+ N -0.23413 0.95812 0.59016
C5+ C -0.18853 0.84076 0.62970
C6+ C -0.19938 0.84377 0.75745
N7+ N -0.25448 0.96292 0.83451
N'8+ N -0.25474 0.94312 0.94692
N'9+ N -0.20004 0.81237 0.93912
N'10+ N -0.16478 0.74806 0.82405
O11+ O -0.12036 0.72898 0.33811
O12+ O -0.30478 1.08915 0.80863
H*13+ H -0.29034 1.07077 0.71766

#END

data_04885_-1.67347E+02
_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 9.726
_cell_length_b 10.004
_cell_length_c 11.607
_cell_angle_alpha 90.00
_cell_angle_beta 138.39
_cell_angle_gamma 90.00
_cell_volume 749.951
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.84463 -0.14709 0.25928
H*2 H 0.80868 -0.06287 0.28351
H*3 H 0.80488 -0.12728 0.15027
N4 N 0.71550 -0.25553 0.21919
H*5 H 0.75048 -0.33835 0.19341
H*6 H 0.75430 -0.27357 0.32741
H*7 H 1.00251 -0.16270 0.36249
N'1+ N 0.24242 0.69311 -0.51657

N'2+ N 0.27005 0.50050 -0.39907
N3+ N 0.26477 0.55892 -0.50741
N'4+ N 0.23287 0.72279 -0.41051
C5+ C 0.24964 0.60669 -0.34223
C6+ C 0.24392 0.60995 -0.22105
N7+ N 0.22209 0.72807 -0.17845
N'8+ N 0.22058 0.70871 -0.06598
N'9+ N 0.24138 0.57925 -0.03943
N'10+ N 0.25618 0.51534 -0.13257
O11+ O 0.27912 0.49540 -0.59157
O12+ O 0.20337 0.85298 -0.23599
H*13+ H 0.20999 0.83459 -0.31806

#END

data_04798_-1.67224E+02
_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 6.989
_cell_length_b 11.913
_cell_length_c 9.539
_cell_angle_alpha 90.00
_cell_angle_beta 72.77
_cell_angle_gamma 90.00
_cell_volume 758.575
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.68707 0.84934 0.51788
H*2 H 0.69370 0.89679 0.60642
H*3 H 0.72229 0.76839 0.53853
N4 N 0.84048 0.88933 0.38957
H*5 H 0.83440 0.84100 0.30252
H*6 H 0.80564 0.97013 0.37080
H*7 H 0.54203 0.85080 0.51170
N'1+ N 0.20268 -0.50925 -0.27402
N'2+ N 0.18099 -0.68937 -0.19737
N3+ N 0.17633 -0.61756 -0.30611
N'4+ N 0.22522 -0.51083 -0.13982
C5+ C 0.21175 -0.61881 -0.09661
C6+ C 0.23116 -0.64486 0.04693

N7+ N 0.26219 -0.56148 0.13474
N'8+ N 0.27558 -0.60337 0.26082
N'9+ N 0.25289 -0.71206 0.25069
N'10+ N 0.22527 -0.74061 0.12076
O11+ O 0.15018 -0.64792 -0.42536
O12+ O 0.27915 -0.44908 0.10698
H*13+ H 0.26265 -0.44424 0.00460

#END

data_07506_-1.66905E+02
_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 4.572
_cell_length_b 15.967
_cell_length_c 10.180
_cell_angle_alpha 90.00
_cell_angle_beta 86.78
_cell_angle_gamma 90.00
_cell_volume 741.978
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.11056 -0.32158 0.57079
H*2 H -0.07256 -0.31263 0.51822
H*3 H 0.11719 -0.38432 0.59337
N4 N 0.07190 -0.27513 0.69271
H*5 H 0.25308 -0.28509 0.74495
H*6 H 0.06225 -0.21300 0.66938
H*7 H 0.29386 -0.30672 0.51145
N'1+ N 0.18468 0.39321 0.00759
N'2+ N 0.53154 0.35389 0.14438
N3+ N 0.36456 0.33146 0.04465
N'4+ N 0.23671 0.45795 0.08598
C5+ C 0.44363 0.43304 0.16640
C6+ C 0.54240 0.49191 0.26275
N7+ N 0.42709 0.57021 0.27072
N'8+ N 0.54746 0.61383 0.36510
N'9+ N 0.73607 0.56262 0.41505
N'10+ N 0.73891 0.48713 0.35459
O11+ O 0.37454 0.26041 -0.00870

O12+ O 0.21800 0.60454 0.19695
H*13+ H 0.17187 0.55669 0.13528

#END

S44. Optimized crystal structure coordinates for 5 polymorphs of **6d** (ionic form).

data_01257_-1.60647E+02
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P 1'
_symmetry_Int_Tables_number 1
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
_cell_length_a 6.965
_cell_length_b 7.139
_cell_length_c 14.120
_cell_angle_alpha 28.68
_cell_angle_beta 90.91
_cell_angle_gamma 70.12
_cell_volume 227.457
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.12337 0.69532 0.24759
N2 N 0.01063 0.19047 0.51183
H*3 H 0.04436 -0.10922 0.60839
H*4 H 0.08207 0.09393 0.62267
N5 N -0.21566 0.81153 0.10590
H*6 H -0.31739 1.19026 -0.09392
H*7 H -0.18636 0.52400 0.19450
N8 N -0.16508 1.08396 0.12504
H*9 H -0.09709 1.00493 0.22830
H*10 H -0.26582 1.46803 -0.07440
N'1+ N 0.13212 1.33441 -0.21389
N'2+ N 0.14507 1.00687 -0.20976
N3+ N 0.06708 1.44787 -0.35787
N'4+ N 0.25661 0.80137 0.03628
C5+ C 0.26182 0.61592 0.03361
C6+ C 0.38707 0.04266 0.28232
N7+ N 0.49591 -0.29526 0.51137
N'8+ N 0.59975 -0.80122 0.71511
N'9+ N 0.55506 -0.77502 0.61200
N'10+ N 0.42477 -0.26281 0.34650
O11+ O -0.05384 1.91741 -0.60475
O12+ O 0.50652 -0.17056 0.54640
H*13+ H 0.41273 0.23657 0.35835

#END

```
data_01878_-1.59948E+02
_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                 12.308
_cell_length_b                 7.094
_cell_length_c                 20.498
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1789.74
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.12325 0.15992 0.24630
N2 N -0.12636 0.00064 0.21145
H*3 H -0.13039 0.00327 0.16221
H*4 H -0.12476 -0.12699 0.23333
N5 N -0.12547 0.32690 0.21604
H*6 H -0.12320 0.44894 0.24144
H*7 H -0.12949 0.33591 0.16690
N8 N -0.11792 0.15222 0.31141
H*9 H -0.11616 0.02756 0.33525
H*10 H -0.11550 0.27084 0.33868
N'1+ N 0.62103 0.50342 -0.11887
N'2+ N 0.62383 0.18550 -0.11434
N3+ N 0.62179 0.34022 -0.15286
N'4+ N 0.62264 0.45286 -0.05612
C5+ C 0.62428 0.26326 -0.05470
C6+ C 0.62625 0.16988 0.00816
N7+ N 0.62642 0.27292 0.06397
N'8+ N 0.62835 0.16026 0.11585
N'9+ N 0.62937 -0.01141 0.09211
N'10+ N 0.62813 -0.01096 0.02611
O11+ O 0.62070 0.33393 -0.21417
O12+ O 0.62491 0.46414 0.07057
H*13+ H 0.62365 0.50858 0.02333
```

```
#END

data_02371_-1.59787E+02
_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                 7.047
_cell_length_b                 6.131
_cell_length_c                 20.730
_cell_angle_alpha               90.00
_cell_angle_beta                82.02
_cell_angle_gamma               90.00
_cell_volume                   886.97
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25514 0.24989 0.50063
N2 N 0.07793 0.25029 0.53356
H*3 H -0.03873 0.25000 0.51018
H*4 H 0.05551 0.25091 0.58278
N5 N 0.28055 0.24908 0.43549
H*6 H 0.41319 0.24876 0.40966
H*7 H 0.16786 0.24876 0.41019
N8 N 0.40694 0.25030 0.53285
H*9 H 0.39096 0.25091 0.58205
H*10 H 0.54205 0.25000 0.50893
N'1+ N 0.02741 -0.25142 0.13810
N'2+ N 0.34755 -0.25103 0.13865
N3+ N 0.20271 -0.25116 0.10214
N'4+ N 0.05960 -0.25148 0.20008
C5+ C 0.25091 -0.25124 0.19914
C6+ C 0.32636 -0.25124 0.26069
N7+ N 0.20531 -0.25148 0.31767
N'8+ N 0.30358 -0.25143 0.36804
N'9+ N 0.48434 -0.25117 0.34220
N'10+ N 0.50382 -0.25105 0.27634
O11+ O 0.22759 -0.25103 0.04089
O12+ O 0.00994 -0.25173 0.32664
H*13+ H -0.02074 -0.25170 0.28006

#END
```

```
data_09594_-1.59765E+02
_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                 20.732
_cell_length_b                 6.133
_cell_length_c                 7.042
_cell_angle_alpha               90.00
_cell_angle_beta                97.95
_cell_angle_gamma                 90.00
_cell_volume                   886.78
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.24931 0.26307 0.24199
N2 N -0.31444 0.26367 0.21690
H*3 H -0.34032 0.26457 0.08430
H*4 H -0.33968 0.26324 0.32981
N5 N -0.21717 0.26366 0.08991
H*6 H -0.16797 0.26322 0.10564
H*7 H -0.24114 0.26456 -0.04518
N8 N -0.21632 0.26188 0.41916
H*9 H -0.23964 0.26142 0.53603
H*10 H -0.16711 0.26141 0.44134
N'1+ N 0.61180 0.25822 -0.47528
N'2+ N 0.61134 0.25822 -0.15491
N3+ N 0.64779 0.26093 -0.30000
N'4+ N 0.54986 0.25360 -0.44282
C5+ C 0.55085 0.25369 -0.25138
C6+ C 0.48935 0.24910 -0.17562
N7+ N 0.43237 0.24483 -0.29653
N'8+ N 0.38205 0.24108 -0.19800
N'9+ N 0.40792 0.24304 -0.01721
N'10+ N 0.47376 0.24796 0.00202
O11+ O 0.70901 0.26551 -0.27534
O12+ O 0.42335 0.24414 -0.49200
H*13+ H 0.46990 0.24761 -0.52289

#END

data_00784_-1.59546E+02
_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 6.221
_cell_length_b 7.126
_cell_length_c 20.444
_cell_angle_alpha 90.00
_cell_angle_beta 89.22
_cell_angle_gamma 90.00
_cell_volume 906.216
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.28112 -0.08803 -0.20764
N2 N 0.28071 0.07853 -0.23778
H*3 H 0.28013 0.08805 -0.28710
H*4 H 0.28096 0.19975 -0.21212
N5 N 0.28077 -0.24621 -0.24284
H*6 H 0.28107 -0.37351 -0.22106
H*7 H 0.28020 -0.24306 -0.29226
N8 N 0.28188 -0.09641 -0.14229
H*9 H 0.28215 0.02137 -0.11476
H*10 H 0.28220 -0.22078 -0.11854
N'1+ N -0.21872 0.25098 0.42588
N'2+ N -0.21881 -0.06550 0.43095
N3+ N -0.21837 0.08804 0.39207
N'4+ N -0.21940 0.20148 0.48888
C5+ C -0.21944 0.01273 0.49063
C6+ C -0.22013 -0.07939 0.55381
N7+ N -0.22072 0.02396 0.60960
N'8+ N -0.22130 -0.08751 0.66181
N'9+ N -0.22106 -0.25875 0.63830
N'10+ N -0.22035 -0.25919 0.57211
O11+ O -0.21771 0.08094 0.33061
O12+ O -0.22077 0.21443 0.61589
H*13+ H -0.22025 0.25804 0.56845

#END

S45. Optimized crystal structure coordinates for 5 polymorphs of **6e** (ionic form).

data_04035_-1.58145E+02
_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                 4.379
_cell_length_b                 24.462
_cell_length_c                 12.249
_cell_angle_alpha               90.00
_cell_angle_beta                132.99
_cell_angle_gamma                 90.00
_cell_volume                   959.767
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.17191 0.66923 0.34240
N2 N -0.16632 0.71671 0.28924
H*3 H -0.16503 0.71778 0.20710
H*4 H -0.16323 0.75282 0.32997
N5 N -0.17589 0.62198 0.28508
H*6 H -0.17463 0.62277 0.20256
N7 N -0.17360 0.66787 0.45050
H*8 H -0.17074 0.70243 0.49626
H*9 H -0.17789 0.63084 0.48665
N10 N -0.18173 0.57251 0.34106
H*11 H -0.44455 0.55099 0.25846
H*12 H 0.07716 0.55008 0.38615
N'1+ N 0.18639 0.36497 -0.05220
N'2+ N 0.19946 0.31755 0.10905
N3+ N 0.19527 0.31520 -0.00227
N'4+ N 0.18476 0.40087 0.02954
C5+ C 0.19263 0.37169 0.12455
C6+ C 0.19279 0.40085 0.22755
N7+ N 0.18513 0.45633 0.22708
N'8+ N 0.18675 0.47474 0.32970
N'9+ N 0.19537 0.43079 0.39308
N'10+ N 0.19930 0.38464 0.33317
O11+ O 0.19920 0.27126 -0.05459
O12+ O 0.17671 0.49139 0.13853
H*13+ H 0.17767 0.46538 0.07385

#END

data_03823_-1.57452E+02
_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                 7.063
_cell_length_b                 11.858
_cell_length_c                 12.153
_cell_angle_alpha               90.00
_cell_angle_beta                107.92
_cell_angle_gamma                 90.00
_cell_volume                   968.472
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.32709 0.28214 0.70067
N2 N 0.29569 0.38856 0.66233
H*3 H 0.31776 0.45436 0.71767
H*4 H 0.24897 0.40593 0.57682
N5 N 0.38935 0.26257 0.81537
H*6 H 0.41180 0.32829 0.87141
N7 N 0.29800 0.19560 0.62778
H*8 H 0.25138 0.20691 0.54123
H*9 H 0.32399 0.11675 0.66139
N10 N 0.42190 0.15123 0.85491
H*11 H 0.56681 0.14037 0.90297
H*12 H 0.33045 0.13149 0.90256
N'1+ N 0.23186 0.13369 0.02934
N'2+ N 0.20569 0.08128 0.20265
N3+ N 0.21327 0.04736 0.09785
N'4+ N 0.23651 0.22686 0.09184
C5+ C 0.22072 0.19352 0.19448
C6+ C 0.22178 0.27881 0.28004
N7+ N 0.23840 0.38953 0.25613
N'8+ N 0.23627 0.45324 0.34587
N'9+ N 0.21841 0.38209 0.42470
N'10+ N 0.20907 0.27416 0.38728
O11+ O 0.20403 -0.05415 0.06670
O12+ O 0.25547 0.43631 0.15714
H*13+ H 0.25250 0.36737 0.10666

#END

data_01224_-1.57252E+02
_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                 11.286
_cell_length_b                 8.028
_cell_length_c                 21.376
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1936.75
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.05980 0.47199 0.38060
N2 N 0.00564 0.41219 0.43165
H*3 H 0.04496 0.32645 0.45934
H*4 H -0.07620 0.45132 0.44389
N5 N 0.16891 0.41659 0.36591
H*6 H 0.20890 0.33048 0.39352
N7 N 0.00798 0.58482 0.34420
H*8 H -0.07374 0.62935 0.35368
H*9 H 0.05290 0.62593 0.30612
N10 N 0.22504 0.47951 0.31253
H*11 H 0.30176 0.53818 0.32454
H*12 H 0.24191 0.38579 0.28167
N'1+ N 0.09819 0.33162 0.01208
N'2+ N 0.26607 0.46166 0.04225
N3+ N 0.21390 0.36023 -0.00009
N'4+ N 0.07445 0.41745 0.06410
C5+ C 0.17561 0.49367 0.08113
C6+ C 0.17490 0.59649 0.13683
N7+ N 0.07391 0.61450 0.17066
N'8+ N 0.09252 0.71340 0.21964
N'9+ N 0.20446 0.75611 0.21599
N'10+ N 0.25789 0.68660 0.16570
O11+ O 0.26715 0.29832 -0.04623
O12+ O -0.03465 0.54607 0.15962
H*13+ H -0.02022 0.47895 0.11991

#END
```

```
data_01915_-1.57015E+02
_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                 11.827
_cell_length_b                 6.947
_cell_length_c                 23.422
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1924.4
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.21409 0.02190 0.64947
N2 N 0.10693 0.03257 0.66775
H*3 H 0.04145 0.03517 0.64005
H*4 H 0.08864 0.03831 0.70984
N5 N 0.23487 0.01450 0.59299
H*6 H 0.16948 0.01706 0.56494
N7 N 0.30019 0.01847 0.68595
H*8 H 0.28798 0.02377 0.72859
H*9 H 0.37964 0.01030 0.66984
N10 N 0.34698 0.00336 0.57415
H*11 H 0.35939 -0.12040 0.55169
H*12 H 0.36622 0.11979 0.54956
N'1+ N 0.63713 -0.21405 0.01368
N'2+ N 0.58565 -0.12257 0.10244
N3+ N 0.55103 -0.16872 0.04914
N'4+ N 0.73086 -0.19672 0.04505
C5+ C 0.69806 -0.14222 0.09763
C6+ C 0.78404 -0.11260 0.14082
N7+ N 0.89483 -0.13969 0.12798
N'8+ N 0.95921 -0.10502 0.17342
N'9+ N 0.88838 -0.05679 0.21406
N'10+ N 0.78001 -0.05988 0.19558
O11+ O 0.44913 -0.16965 0.03382
O12+ O 0.94111 -0.19429 0.07719
```

```
H*13+ H 0.87174 -0.20917 0.05182

#END

data_00098_-1.56945E+02
_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                 6.827
_cell_length_b                 13.257
_cell_length_c                 21.419
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1938.54
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.21693 0.58576 0.37403
N2 N 0.29330 0.57454 0.43123
H*3 H 0.27530 0.51003 0.45569
H*4 H 0.37116 0.63042 0.45152
N5 N 0.11406 0.50943 0.34864
H*6 H 0.09544 0.44444 0.37296
N7 N 0.24071 0.67068 0.34189
H*8 H 0.31688 0.72956 0.35936
H*9 H 0.17984 0.67522 0.29879
N10 N 0.03465 0.52159 0.28888
H*11 H 0.09145 0.46926 0.25914
H*12 H -0.11400 0.51547 0.29047
N'1+ N 0.21572 0.40402 0.50276
N'2+ N 0.11540 0.24206 0.50880
N3+ N 0.14167 0.32372 0.47190
N'4+ N 0.23828 0.37342 0.56172
C5+ C 0.17766 0.27693 0.56413
C6+ C 0.18640 0.22456 0.62344
N7+ N 0.25448 0.27258 0.67504
N'8+ N 0.25016 0.21126 0.72420
```

N'9+ N 0.17973 0.12585 0.70298
N'10+ N 0.13888 0.13123 0.64125
O11+ O 0.10156 0.32530 0.41461
O12+ O 0.32061 0.36927 0.68012
H*13+ H 0.30570 0.39555 0.63570

#END

S46. Optimized crystal structure coordinates for 5 polymorphs of **6f** (ionic form).

data_01814_-1.52432E+02
_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 4.056
_cell_length_b 11.536
_cell_length_c 21.903
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1024.84
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.05418 -0.18029 0.26829
N2 N 0.08073 -0.24916 0.31067
H*3 H 0.22336 -0.31606 0.29601
N4 N 0.00392 -0.20223 0.20882
H*5 H -0.09722 -0.15053 0.17638
N6 N -0.24340 -0.09124 0.28484
H*7 H -0.28037 -0.07802 0.33009
H*8 H -0.34810 -0.03798 0.25385
N9 N 0.20396 -0.29654 0.19307
N10 N 0.01943 -0.22591 0.37244
H*11 H 0.23568 -0.20961 0.39446
H*12 H 0.07462 -0.35442 0.16742
H*13 H 0.40642 -0.26884 0.16978
H*14 H -0.09534 -0.29499 0.39211
N'1+ N 0.12873 0.58512 -0.12327
N'2+ N -0.19523 0.43900 -0.09006
N3+ N -0.02728 0.48521 -0.13752
N'4+ N 0.05962 0.60441 -0.06453
C5+ C -0.13321 0.51640 -0.04582
C6+ C -0.24580 0.51567 0.01696

N7+ N -0.15703 0.60230 0.05555
N'8+ N -0.28609 0.58500 0.11066
N'9+ N -0.45358 0.48815 0.10602
N'10+ N -0.43442 0.44310 0.04909
O11+ O -0.01630 0.44022 -0.18977
O12+ O 0.03517 0.69657 0.04361
H*13+ H 0.09366 0.68504 -0.00119

#END

data_01729_-1.51438E+02
_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 4.092
_cell_length_b 11.887
_cell_length_c 22.328
_cell_angle_alpha 90.00
_cell_angle_beta 72.86
_cell_angle_gamma 90.00
_cell_volume 1037.83
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.66931 0.29103 -0.37961
N2 N 0.73364 0.28572 -0.32426
H*3 H 0.85119 0.35283 -0.31130
N4 N 0.76176 0.38378 -0.41531
H*5 H 0.71408 0.38858 -0.45732
N6 N 0.51579 0.20555 -0.39903
H*7 H 0.45080 0.13748 -0.37063
H*8 H 0.46428 0.20735 -0.44053
N9 N 0.92261 0.47201 -0.39345
N10 N 0.63693 0.18906 -0.28734
H*11 H 0.46712 0.20985 -0.24541
H*12 H 1.16035 0.48568 -0.42340
H*13 H 0.77961 0.54338 -0.38859
H*14 H 0.84697 0.15229 -0.28013
N'1+ N -0.36180 -0.21006 0.51370
N'2+ N -0.36775 -0.30733 0.60085
N3+ N -0.44037 -0.30785 0.54555
N'4+ N -0.23377 -0.14379 0.54956

```
C5+ C -0.23997 -0.20348 0.60108
C6+ C -0.11378 -0.15097 0.64849
N7+ N 0.00724 -0.04397 0.64056
N'8+ N 0.10969 -0.01217 0.68927
N'9+ N 0.05203 -0.09920 0.72704
N'10+ N -0.08520 -0.18604 0.70352
O11+ O -0.56815 -0.39068 0.52551
O12+ O 0.03021 0.02683 0.59145
H*13+ H -0.06587 -0.02099 0.56274

#END

data_04841_-1.51110E+02
_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                 4.413
_cell_length_b                 13.092
_cell_length_c                 18.893
_cell_angle_alpha               90.00
_cell_angle_beta                73.11
_cell_angle_gamma                 90.00
_cell_volume                   1044.46
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 1.00235 0.52735 0.21932
N2 N 0.86189 0.45816 0.18717
H*3 H 0.78191 0.39289 0.21564
N4 N 1.03141 0.50786 0.28710
H*5 H 1.13747 0.55981 0.31189
N6 N 1.11180 0.61431 0.18461
H*7 H 1.08477 0.62573 0.13371
H*8 H 1.21862 0.66776 0.20757
N9 N 0.91368 0.41569 0.32195
N10 N 0.83235 0.47885 0.11670
H*11 H 0.59930 0.47983 0.11865
H*12 H 1.09204 0.37399 0.33176
H*13 H 0.74205 0.42943 0.37023
H*14 H 0.94847 0.42452 0.08027
N'1+ N -0.63472 0.64079 0.35203
N'2+ N -0.37349 0.78785 0.35630
```

```
N3+ N -0.53236 0.73104 0.31899
N'4+ N -0.53898 0.63898 0.41289
C5+ C -0.38430 0.72720 0.41420
C6+ C -0.25381 0.74540 0.47514
N7+ N -0.28844 0.67446 0.52932
N'8+ N -0.15194 0.70615 0.57962
N'9+ N -0.03376 0.79619 0.55652
N'10+ N -0.09180 0.82280 0.49248
O11+ O -0.58082 0.75890 0.25951
O12+ O -0.43742 0.58222 0.53580
H*13+ H -0.51466 0.58060 0.48999

#END

data_04128_-1.51107E+02
_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                 18.386
_cell_length_b                 13.089
_cell_length_c                 4.414
_cell_angle_alpha               90.00
_cell_angle_beta                100.48
_cell_angle_gamma               90.00
_cell_volume                   1044.53
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.78066 0.47263 0.05908
N2 N 0.81280 0.54181 0.26391
H*3 H 0.78433 0.60707 0.28703
N4 N 0.71288 0.49212 -0.10552
H*5 H 0.68809 0.44016 -0.26123
N6 N 0.81538 0.38567 0.01896
H*7 H 0.86629 0.37425 0.14778
H*8 H 0.79243 0.33223 -0.13383
N9 N 0.67801 0.58428 -0.05742
N10 N 0.88328 0.52112 0.43437
H*11 H 0.88134 0.52009 0.66346
H*12 H 0.66819 0.62602 -0.25528
H*13 H 0.62975 0.57050 0.01758
H*14 H 0.91970 0.57548 0.39124
```

N'1+ N -0.14800 0.85918 -0.43060
N'2+ N -0.14375 0.71214 -0.16065
N3+ N -0.18106 0.76894 -0.39420
N'4+ N -0.08714 0.86101 -0.21316
C5+ C -0.08584 0.77280 -0.05576
C6+ C -0.02489 0.75462 0.19662
N7+ N 0.02930 0.82556 0.27026
N'8+ N 0.07960 0.79389 0.50738
N'9+ N 0.05649 0.70385 0.57947
N'10+ N -0.00755 0.67723 0.39341
O11+ O -0.24054 0.74107 -0.56157
O12+ O 0.03579 0.91779 0.13413
H*13+ H -0.01002 0.91940 -0.03471

#END

data_07604_-1.51071E+02
_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 14.017
_cell_length_b 6.810
_cell_length_c 10.389
_cell_angle_alpha 90.00
_cell_angle_beta 100.16
_cell_angle_gamma 90.00
_cell_volume 976.139
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.13243 0.85425 -0.79323
N2 N -0.18426 0.90274 -0.70135
H*3 H -0.14783 0.92345 -0.60871
N4 N -0.03552 0.83520 -0.75953
H*5 H 0.00435 0.79851 -0.82846
N6 N -0.17630 0.82528 -0.91634
H*7 H -0.24932 0.84121 -0.93722
H*8 H -0.13899 0.78863 -0.98750
N9 N 0.00818 0.86672 -0.62924
N10 N -0.28499 0.92233 -0.73698
H*11 H -0.30522 1.06157 -0.71818
H*12 H 0.04249 0.74262 -0.59090

H*13 H 0.05607 0.98016 -0.62323
H*14 H -0.31878 0.82460 -0.68592
N'1+ N 0.14566 0.56645 -0.47605
N'2+ N 0.23481 0.59225 -0.27340
N3+ N 0.23483 0.55640 -0.40143
N'4+ N 0.08570 0.61034 -0.39359
C5+ C 0.14039 0.62491 -0.27377
C6+ C 0.09304 0.67194 -0.16443
N7+ N -0.00430 0.70032 -0.18373
N'8+ N -0.03281 0.74171 -0.07120
N'9+ N 0.04662 0.73884 0.01702
N'10+ N 0.12538 0.69647 -0.03671
O11+ O 0.30997 0.51754 -0.44713
O12+ O -0.06906 0.69078 -0.29807
H*13+ H -0.02583 0.65729 -0.36413

#END

S47. Optimized crystal structure coordinates for 5 polymorphs of **6g** (ionic form).

data_04391_-1.47861E+02
_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 7.543
_cell_length_b 19.746
_cell_length_c 7.326
_cell_angle_alpha 90.00
_cell_angle_beta 98.50
_cell_angle_gamma 90.00
_cell_volume 1079.18
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.44473 0.31608 0.85265
N2 N 0.32575 0.36429 0.79070
H*3 H 0.25135 0.35730 0.66467
N4 N 0.54626 0.32280 1.01801
H*5 H 0.52897 0.36518 1.09216
N6 N 0.46218 0.26115 0.74924
H*7 H 0.55387 0.22576 0.80112
N8 N 0.66962 0.27169 1.07962
N9 N 0.31008 0.42122 0.90142
H*10 H 0.18316 0.42434 0.93261

H*11 H 0.79613 0.29107 1.10069
H*12 H 0.64011 0.25145 1.19940
H*13 H 0.33917 0.46396 0.83390
N14 N 0.35449 0.25533 0.57692
H*15 H 0.43291 0.25264 0.47529
H*16 H 0.27690 0.21302 0.57400
N'1+ N 0.01912 0.41527 0.14365
N'2+ N 0.13926 0.40364 0.44302
N3+ N 0.04845 0.37364 0.29142
N'4+ N 0.09347 0.47433 0.20135
C5+ C 0.16398 0.46615 0.37968
C6+ C 0.25406 0.52316 0.47761
N7+ N 0.26612 0.58317 0.38990
N'8+ N 0.35348 0.62843 0.50416
N'9+ N 0.39502 0.59644 0.66154
N'10+ N 0.33608 0.53164 0.65039
O11+ O -0.00384 0.31312 0.28737
O12+ O 0.20217 0.59932 0.21136
H*13+ H 0.14387 0.55518 0.16193

#END

data_01008_-1.46274E+02
_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 12.988
_cell_length_b 8.575
_cell_length_c 10.459
_cell_angle_alpha 90.00
_cell_angle_beta 85.62
_cell_angle_gamma 90.00
_cell_volume 1161.44
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.48778 -0.03032 0.17199
N2 N 0.46391 0.12178 0.17694
H*3 H 0.52227 0.19869 0.18714
N4 N 0.41370 -0.13666 0.15861
H*5 H 0.34042 -0.09723 0.15256
N6 N 0.58573 -0.07608 0.18042

H*7 H 0.60064 -0.19242 0.17626
N8 N 0.44065 -0.29491 0.15369
N9 N 0.36096 0.16659 0.16792
H*10 H 0.35545 0.23644 0.08999
H*11 H 0.40202 -0.35328 0.22737
H*12 H 0.42289 -0.34169 0.06862
H*13 H 0.33458 0.22485 0.24874
N14 N 0.66173 0.03735 0.19436
H*15 H 0.69544 0.02009 0.27799
H*16 H 0.71631 0.03168 0.11924
N'1+ N 0.09930 0.10795 0.13068
N'2+ N 0.18089 -0.10896 0.19192
N3+ N 0.14914 -0.02455 0.09303
N'4+ N 0.09869 0.10957 0.25841
C5+ C 0.14763 -0.02053 0.29250
C6+ C 0.15812 -0.04841 0.42753
N7+ N 0.11913 0.05524 0.51663
N'8+ N 0.13704 0.00766 0.63397
N'9+ N 0.18682 -0.12471 0.61722
N'10+ N 0.20116 -0.16284 0.49159
O11+ O 0.16420 -0.06460 -0.02254
O12+ O 0.06802 0.19114 0.49753
H*13+ H 0.06682 0.19432 0.40033

#END

data_09590_-1.46172E+02
_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 15.062
_cell_length_b 7.145
_cell_length_c 10.933
_cell_angle_alpha 90.00
_cell_angle_beta 112.97
_cell_angle_gamma 90.00
_cell_volume 1083.3
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.17784 0.10051 0.37439
N2 N 0.15967 0.19776 0.46692

H*3 H 0.21471 0.27296 0.53332
N4 N 0.10777 -0.00101 0.28443
H*5 H 0.04188 -0.00059 0.28974
N6 N 0.26608 0.10479 0.37182
H*7 H 0.27693 0.02916 0.30011
N8 N 0.12860 -0.10141 0.18874
N9 N 0.06685 0.19098 0.46748
H*10 H 0.03786 0.32187 0.45426
H*11 H 0.11761 -0.24062 0.19716
H*12 H 0.08568 -0.05637 0.09606
H*13 H 0.06979 0.13763 0.55536
N14 N 0.33807 0.21197 0.46694
H*15 H 0.39402 0.12815 0.52231
H*16 H 0.36208 0.31240 0.42121
N'1+ N 0.51636 0.04357 -0.15882
N'2+ N 0.65647 0.02715 -0.18806
N3+ N 0.55927 0.03888 -0.24667
N'4+ N 0.58819 0.03457 -0.03907
C5+ C 0.67073 0.02491 -0.05906
C6+ C 0.76103 0.01375 0.05575
N7+ N 0.76137 0.01317 0.18009
N'8+ N 0.85118 0.00218 0.27058
N'9+ N 0.90592 -0.00399 0.20227
N'10+ N 0.85300 0.00283 0.06995
O11+ O 0.51301 0.04488 -0.37038
O12+ O 0.68454 0.02209 0.21637
H*13+ H 0.62773 0.02918 0.12699

#END

data_01368_-1.45203E+02
_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 7.415
_cell_length_b 10.113
_cell_length_c 13.445
_cell_angle_alpha 39.56
_cell_angle_beta 59.65
_cell_angle_gamma 67.95
_cell_volume 553.934
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

```
C1 C -0.46268 -0.20263 0.34421
N2 N -0.28270 -0.17834 0.33018
H*3 H -0.29072 -0.17194 0.40415
N4 N -0.46089 -0.21203 0.24956
H*5 H -0.31991 -0.20013 0.16871
N6 N -0.64445 -0.21752 0.45289
H*7 H -0.77741 -0.23582 0.45977
N8 N -0.65112 -0.23748 0.26658
N9 N -0.09482 -0.16317 0.21567
H*10 H 0.00003 -0.28084 0.27727
H*11 H -0.67286 -0.11445 0.15519
H*12 H -0.65133 -0.37122 0.30378
H*13 H -0.02150 -0.02407 0.12868
N14 N -0.64211 -0.20724 0.55038
H*15 H -0.72598 -0.08422 0.52588
H*16 H -0.70445 -0.34099 0.67446
N'1+ N 0.25001 0.45941 -0.09617
N'2+ N 0.18337 0.16645 0.18015
N3+ N 0.20888 0.25267 0.03199
N'4+ N 0.25122 0.50906 -0.02886
C5+ C 0.21124 0.33237 0.13545
C6+ C 0.20338 0.34178 0.23978
N7+ N 0.23588 0.52560 0.17179
N'8+ N 0.22184 0.49981 0.28865
N'9+ N 0.18088 0.30099 0.42799
N'10+ N 0.16840 0.19900 0.40274
O11+ O 0.19587 0.15161 0.01435
O12+ O 0.27774 0.71628 0.00911
H*13+ H 0.27818 0.68492 -0.04707

#END

data_01088_-1.45069E+02
_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                 7.297
_cell_length_b                 10.924
_cell_length_c                 13.675
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1090.07
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.10790 -0.16141 0.56468
N2 N -0.20842 -0.26134 0.58368
H*3 H -0.28611 -0.29584 0.52847
N4 N -0.00301 -0.11221 0.63492
H*5 H -0.00349 -0.15339 0.70158
N6 N -0.11227 -0.11068 0.47544
H*7 H -0.03410 -0.03500 0.46399
N8 N 0.10077 -0.00776 0.61321
N9 N -0.20147 -0.31262 0.67753
H*10 H -0.15447 -0.40027 0.67370
H*11 H 0.06234 0.06271 0.65744
H*12 H 0.23650 -0.02573 0.62293
H*13 H -0.32863 -0.31183 0.70821
N14 N -0.22300 -0.16385 0.40330
H*15 H -0.31865 -0.10245 0.38016
H*16 H -0.14449 -0.19089 0.34564
N'1+ N 0.04992 0.22268 0.26170
N'2+ N 0.04667 0.11332 0.40176
N3+ N 0.05701 0.11044 0.30304
N'4+ N 0.03445 0.30111 0.33615
C5+ C 0.03282 0.23392 0.41860
C6+ C 0.01703 0.29684 0.51150
N7+ N 0.00428 0.42076 0.51428
N'8+ N -0.00900 0.45969 0.60621
N'9+ N -0.00444 0.36018 0.65980
N'10+ N 0.01148 0.25838 0.60409
O11+ O 0.07174 0.01343 0.25418
O12+ O 0.00398 0.50094 0.43788
H*13+ H 0.01567 0.44424 0.37910

#END
```

S48. Optimized crystal structure coordinates for 5 polymorphs of **7a** (ionic form).

```
data_2NH4_BTO_0_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                 7.391
_cell_length_b                 18.130
_cell_length_c                 3.847
_cell_angle_alpha               46.12
_cell_angle_beta                109.21
_cell_angle_gamma                 114.64
_cell_volume                   337.1
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.30561 0.39268 0.47619
H*2 H -0.17491 0.39513 0.42357
H*3 H -0.29160 0.46397 0.37673
H*4 H -0.42028 0.37958 0.26967
H*5 H -0.33565 0.33204 0.83479
N1 N -0.30543 0.89310 -0.02769
H*2 H -0.41987 0.88039 -0.23570
H*3 H -0.29176 0.96404 -0.12425
H*4 H -0.33558 0.83199 0.33067
H*5 H -0.17452 0.89597 -0.08148
N'1+ N -0.24871 0.07706 0.77456
N'2+ N -0.25937 0.23009 0.48382
N'3+ N -0.36072 0.14372 0.52188
N'4+ N -0.07132 0.11819 0.90803
C5+ C -0.08124 0.21262 0.72472
C6+ C 0.08090 0.28678 0.78022
N'7+ N 0.25903 0.26931 1.02112
N'8+ N 0.36038 0.35568 0.98306
N'9+ N 0.24837 0.42234 0.73038
N'10+ N 0.07098 0.38121 0.59691

#END

data_2NH4_BTO_0_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'C 2/c'
_symmetry_Int_Tables_number      15
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z
_cell_length_a                 15.941
_cell_length_b                 3.961
_cell_length_c                 21.605
_cell_angle_alpha               90.00
_cell_angle_beta                94.13
_cell_angle_gamma                90.00
_cell_volume                   1360.65
loop_
```

```
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.37857 0.20693 -0.77436
H*2 H 0.41291 0.01319 -0.79159
H*3 H 0.41874 0.38289 -0.75356
H*4 H 0.34251 0.31861 -0.81004
H*5 H 0.34012 0.11303 -0.74225
N1 N 0.36932 0.18582 -0.97780
H*2 H 0.33041 0.00510 -0.99846
H*3 H 0.40852 0.07600 -0.94369
H*4 H 0.40468 0.29329 -1.01053
H*5 H 0.33367 0.36889 -0.95852
N'1+ N 0.47479 0.84064 0.10397
N'2+ N 0.54779 0.59535 0.18084
N'3+ N 0.47965 0.78522 0.16481
N'4+ N 0.53963 0.68841 0.07871
C5+ C 0.58383 0.53866 0.12699
C6+ C 0.66119 0.33966 0.12161
N'7+ N 0.69723 0.28297 0.06776
N'8+ N 0.76537 0.09310 0.08379
N'9+ N 0.77023 0.03768 0.14463
N'10+ N 0.70539 0.18991 0.16989

#END

data_2NH4_BTO_0_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                 19.880
_cell_length_b                 10.895
_cell_length_c                 3.708
_cell_angle_alpha               90.00
_cell_angle_beta                58.28
_cell_angle_gamma                 90.00
_cell_volume                   683.161
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

N1 N 0.62507 0.45468 0.75094
H*2 H 0.58829 0.40020 0.70270
H*3 H 0.66188 0.40023 0.79904
H*4 H 0.65836 0.50918 0.48932
H*5 H 0.59175 0.50911 1.01271
N1 N 0.62508 0.04525 0.75079
H*2 H 0.65838 -0.00925 0.48918
H*3 H 0.59174 -0.00919 1.01252
H*4 H 0.66187 0.09969 0.79904
H*5 H 0.58832 0.09974 0.70242
N'1+ N 0.22809 0.18907 0.83528
N'2+ N 0.29538 0.35245 0.79660
N'3+ N 0.22808 0.31106 0.83554
N'4+ N 0.29540 0.14764 0.79617
C5+ C 0.33600 0.25004 0.77284
C6+ C 0.41430 0.25002 0.72744
N'7+ N 0.45492 0.14761 0.70368
N'8+ N 0.52222 0.18900 0.66474
N'9+ N 0.52221 0.31099 0.66500
N'10+ N 0.45490 0.35242 0.70411

#END

data_2NH4_BTO_0_4
_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 13.690
_cell_length_b 6.951
_cell_length_c 3.669
_cell_angle_alpha 90.00
_cell_angle_beta 82.59
_cell_angle_gamma 90.00
_cell_volume 346.223
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.89910 0.30279 -0.40312
H*2 H 0.83849 0.28349 -0.53780
H*3 H 0.90371 0.19138 -0.22192
H*4 H 0.96160 0.30559 -0.59125
H*5 H 0.89261 0.43071 -0.26151
N1 N 0.60078 0.60760 -0.09737
H*2 H 0.59610 0.71903 -0.27848

H*3 H 0.66145 0.62689 0.03698
H*4 H 0.53834 0.60479 0.09105
H*5 H 0.60723 0.47969 -0.23902
N'1+ N 0.12897 0.15346 1.08367
N'2+ N 0.12034 0.46277 0.98525
N'3+ N 0.07131 0.30763 1.13236
N'4+ N 0.21714 0.20395 0.90352
C5+ C 0.21014 0.39540 0.84564
C6+ C 0.28994 0.51502 0.65528
N'7+ N 0.37974 0.44765 0.51567
N'8+ N 0.42877 0.60279 0.36856
N'9+ N 0.37111 0.75696 0.41725
N'10+ N 0.28294 0.70647 0.59740

#END

data_2NH4_BTO_0_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 15.544
_cell_length_b 7.827
_cell_length_c 3.961
_cell_angle_alpha 54.56
_cell_angle_beta 59.31
_cell_angle_gamma 65.18
_cell_volume 332.316
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.40936 -0.19509 0.32021
H*2 H 0.43943 -0.11038 -0.02026
H*3 H 0.34283 -0.10646 0.44073
H*4 H 0.39486 -0.33515 0.40875
H*5 H 0.46032 -0.22838 0.45162
N1 N 0.09056 0.69309 0.68737
H*2 H 0.15703 0.60031 0.57963
H*3 H 0.05805 0.61312 1.02780
H*4 H 0.10587 0.83346 0.59318
H*5 H 0.04129 0.72547 0.54887
N'1+ N 0.12529 0.04201 0.56575
N'2+ N 0.11685 0.34274 0.51038
N'3+ N 0.06625 0.22711 0.54326
N'4+ N 0.21598 0.03199 0.54812

C5+ C 0.20905 0.21923 0.51401
C6+ C 0.29123 0.28067 0.48463
N'7+ N 0.38343 0.15716 0.48826
N'8+ N 0.43403 0.27279 0.45538
N'9+ N 0.37499 0.45789 0.43289
N'10+ N 0.28430 0.46791 0.45052

#END

S49. Optimized crystal structure coordinates for 5 polymorphs of **7b** (ionic form).

data_2NH3OH_BTO_0_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 9.412
_cell_length_b 13.280
_cell_length_c 8.480
_cell_angle_alpha 90.00
_cell_angle_beta 128.93
_cell_angle_gamma 90.00
_cell_volume 824.532
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.15892 0.34871 0.49364
H*2 H 0.25822 0.33811 0.47837
H*3 H 0.07997 0.40997 0.40714
H*4 H 0.08016 0.28435 0.44607
O5 O 0.25647 0.36640 0.70177
H*6 H 0.16681 0.37690 0.72292
N1 N -0.15893 0.84871 0.00633
H*2 H -0.25822 0.83810 0.02163
H*3 H -0.07999 0.90997 0.09283
H*4 H -0.08016 0.78435 0.05390
O5 O -0.25651 0.86639 -0.20180
H*6 H -0.16687 0.87690 -0.22297
N'1+ N 0.01463 -0.16771 0.63690
N'2+ N 0.08049 -0.02337 0.79288
N'3+ N -0.02306 -0.10685 0.73074
N'4+ N 0.14375 -0.12554 0.63534
C5+ C 0.18233 -0.03654 0.73238
C6+ C 0.31767 0.03654 0.76762
N'7+ N 0.41951 0.02337 0.70712

N'8+ N 0.52306 0.10685 0.76926
N'9+ N 0.48537 0.16771 0.86310
N'10+ N 0.35625 0.12554 0.86466

#END

data_2NH3OH_BTO_0_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 16.325
_cell_length_b 3.912
_cell_length_c 13.594
_cell_angle_alpha 90.00
_cell_angle_beta 106.48
_cell_angle_gamma 90.00
_cell_volume 832.494
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.12094 0.17815 0.14760
H*2 H 0.18113 0.27249 0.15372
H*3 H 0.10377 0.01276 0.08592
H*4 H 0.12194 0.05324 0.21488
O5 O 0.06816 0.46875 0.13205
H*6 H 0.01012 0.39010 0.12582
N1 N 0.62096 0.17811 0.14768
H*2 H 0.68116 0.27247 0.15384
H*3 H 0.60381 0.01279 0.08598
H*4 H 0.62193 0.05312 0.21493
O5 O 0.56818 0.46871 0.13212
H*6 H 0.51014 0.39005 0.12584
N'1+ N 0.09120 0.80186 0.39163
N'2+ N 0.21976 0.73814 0.37545
N'3+ N 0.14152 0.86885 0.33242
N'4+ N 0.13527 0.62568 0.47486
C5+ C 0.21443 0.58932 0.46326
C6+ C 0.28557 0.41080 0.53670
N'7+ N 0.28024 0.26198 0.62451
N'8+ N 0.35848 0.13127 0.66754
N'9+ N 0.40880 0.19826 0.60833
N'10+ N 0.36473 0.37444 0.52510

#END

data_2NH3OH_BTO_0_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 26.139
_cell_length_b 8.168
_cell_length_c 3.905
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 833.731
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.80105 0.05720 0.31912
H*2 H 0.79773 0.17383 0.41744
H*3 H 0.76761 0.02765 0.19251
H*4 H 0.83188 0.05391 0.15371
O5 O 0.80893 -0.04296 0.60713
H*6 H 0.81230 -0.15533 0.52468
N1 N 0.05104 0.28974 0.46357
H*2 H 0.04808 0.40692 0.36764
H*3 H 0.08181 0.28474 0.62926
H*4 H 0.01747 0.26058 0.58916
O5 O 0.05871 0.19072 0.17358
H*6 H 0.06173 0.07786 0.25373
N'1+ N -0.20864 0.52113 0.50780
N'2+ N -0.13766 0.60078 0.26330
N'3+ N -0.17924 0.64975 0.43885
N'4+ N -0.18702 0.38485 0.37906
C5+ C -0.14327 0.43692 0.22936
C6+ C -0.10651 0.32916 0.05236
N'7+ N -0.11212 0.16530 0.01842
N'8+ N -0.07054 0.11633 -0.15713
N'9+ N -0.04114 0.24495 -0.22608
N'10+ N -0.06276 0.38123 -0.09734

#END

```
data_2NH3OH_BTO_0_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a                 6.923
_cell_length_b                 8.162
_cell_length_c                 13.209
_cell_angle_alpha               90.00
_cell_angle_beta                81.58
_cell_angle_gamma                 90.00
_cell_volume                   738.336
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.16897 0.97215 0.64582
H*2 H -0.06090 1.05867 0.64704
H*3 H -0.15062 0.91640 0.57485
H*4 H -0.15928 0.88734 0.70290
O5 O -0.34421 1.06156 0.66385
H*6 H -0.45107 0.98359 0.66331
N1 N 0.16898 0.52785 0.35419
H*2 H 0.06088 0.44136 0.35294
H*3 H 0.15936 0.61269 0.29711
H*4 H 0.15058 0.58358 0.42516
O5 O 0.34419 0.43841 0.33618
H*6 H 0.45107 0.51635 0.33676
N'1+ N 0.21839 0.20341 0.17774
N'2+ N 0.24922 0.33825 0.03331
N'3+ N 0.13012 0.30563 0.12094
N'4+ N 0.39741 0.16663 0.12867
C5+ C 0.41327 0.25119 0.03975
C6+ C 0.58669 0.24877 -0.03977
N'7+ N 0.75074 0.16171 -0.03333
N'8+ N 0.86984 0.19433 -0.12096
N'9+ N 0.78157 0.29655 -0.17776
N'10+ N 0.60255 0.33333 -0.12869

#END

data_2NH3OH_BTO_0_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                13.935
_cell_length_b                8.304
_cell_length_c                13.384
_cell_angle_alpha              90.00
_cell_angle_beta               80.98
_cell_angle_gamma                90.00
_cell_volume                  1529.59
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.13007 0.57114 0.85115
H*2 H -0.05658 0.59448 0.84231
H*3 H -0.16310 0.62156 0.91838
H*4 H -0.15774 0.61980 0.79058
O5 O -0.13681 0.40222 0.85285
H*6 H -0.20577 0.37482 0.86117
N1 N 0.33007 0.51212 0.85610
H*2 H 0.27908 0.42198 0.85715
H*3 H 0.32283 0.59106 0.79810
H*4 H 0.31898 0.57057 0.92508
O5 O 0.41995 0.43171 0.83930
H*6 H 0.47060 0.51335 0.83777
N'1+ N -0.19003 0.72617 0.12464
N'2+ N -0.05220 0.84670 0.13365
N'3+ N -0.14341 0.82101 0.18109
N'4+ N -0.13046 0.68748 0.03888
C5+ C -0.04583 0.76317 0.04607
C6+ C 0.04187 0.75561 -0.03143
N'7+ N 0.04824 0.67208 -0.11901
N'8+ N 0.13945 0.69777 -0.16645
N'9+ N 0.18607 0.79261 -0.11000
N'10+ N 0.12650 0.83130 -0.02424

#END
```

S50. Optimized crystal structure coordinates for 5 polymorphs of **7c** (ionic form).

```
data_2N2H5_BTO_0_1
_symmetry_cell_setting          monoclinic
```

```
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a                   16.258
_cell_length_b                   4.845
_cell_length_c                   12.672
_cell_angle_alpha                 90.00
_cell_angle_beta                  108.16
_cell_angle_gamma                    90.00
_cell_volume                     948.454
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.08403 0.34954 0.39298
H*2 H 0.01991 0.31222 0.38397
H*3 H 0.08566 0.44783 0.32170
N4 N 0.12746 0.08622 0.39932
H*5 H 0.19083 0.12505 0.40700
H*6 H 0.12471 -0.01134 0.46962
H*7 H 0.10870 0.48108 0.45949
N1 N 0.58403 0.34954 -0.10701
H*2 H 0.51992 0.31224 -0.11601
H*3 H 0.58566 0.44783 -0.17829
N4 N 0.62745 0.08619 -0.10069
H*5 H 0.69082 0.12499 -0.09302
H*6 H 0.62470 -0.01138 -0.03039
H*7 H 0.60872 0.48105 -0.04050
N'1+ N 0.13441 -0.31120 0.57517
N'2+ N 0.13193 -0.07303 0.72063
N'3+ N 0.08455 -0.22498 0.63410
N'4+ N 0.21565 -0.21778 0.62169
C5+ C 0.21259 -0.07137 0.71131
C6+ C 0.28741 0.07135 0.78871
N'7+ N 0.36807 0.07301 0.77939
N'8+ N 0.41545 0.22496 0.86592
N'9+ N 0.36559 0.31118 0.92485
N'10+ N 0.28435 0.21776 0.87833

#END

data_2N2H5_BTO_0_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                   7.078
_cell_length_b                   14.903
_cell_length_c                   9.394
_cell_angle_alpha                 90.00
_cell_angle_beta                  125.54
_cell_angle_gamma                   90.00
_cell_volume                     806.314
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.13726 0.61880 0.02124
H*2 H 0.21866 0.56851 0.11287
H*3 H 0.19207 0.61326 -0.05860
N4 N 0.21772 0.70407 0.11153
H*5 H 0.13813 0.75362 0.01950
H*6 H 0.16486 0.70861 0.19195
H*7 H -0.03983 0.60813 -0.05277
N1 N 0.36272 0.11879 -0.02123
H*2 H 0.28132 0.06849 -0.11285
H*3 H 0.30792 0.11326 0.05861
N4 N 0.28228 0.20406 -0.11154
H*5 H 0.36188 0.25361 -0.01952
H*6 H 0.33513 0.20859 -0.19197
H*7 H 0.53982 0.10812 0.05278
N'1+ N -0.57308 0.35582 0.08753
N'2+ N -0.53090 0.48161 0.22282
N'3+ N -0.66823 0.40967 0.14240
N'4+ N -0.37115 0.39120 0.13071
C5+ C -0.34866 0.46879 0.21405
C6+ C -0.15132 0.53121 0.28595
N'7+ N 0.03092 0.51839 0.27718
N'8+ N 0.16825 0.59033 0.35760
N'9+ N 0.07310 0.64418 0.41247
N'10+ N -0.12883 0.60880 0.36929

#END

data_2N2H5_BTO_0_3
_symmetry_cell_setting           monoclinic
_symmetry_space_group_name_H-M   'C 2'
_symmetry_Int_Tables_number      5
```

```
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,-z
3 1/2+x,1/2+y,z
4 1/2-x,1/2+y,-z
_cell_length_a                 13.358
_cell_length_b                 4.921
_cell_length_c                 12.868
_cell_angle_alpha               90.00
_cell_angle_beta                108.58
_cell_angle_gamma                 90.00
_cell_volume                   801.787
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.40179 -0.05388 -0.41184
H*2 H 0.39716 0.03811 -0.48501
H*3 H 0.46394 0.03561 -0.35281
N4 N 0.42718 -0.33780 -0.41929
H*5 H 0.43280 -0.42694 -0.34594
H*6 H 0.36564 -0.42442 -0.47889
H*7 H 0.33306 -0.01439 -0.39408
N1 N -0.09821 0.28541 0.08816
H*2 H -0.03607 0.19591 0.14719
H*3 H -0.10285 0.19341 0.01500
N4 N -0.07282 0.56932 0.08071
H*5 H -0.13435 0.65596 0.02111
H*6 H -0.06719 0.65846 0.15406
H*7 H -0.16695 0.24594 0.10592
N'1+ N 0.08712 -0.28278 0.68575
N'2+ N 0.20881 -0.10765 0.62587
N'3+ N 0.12957 -0.28931 0.60535
N'4+ N 0.13754 -0.09668 0.76084
C5+ C 0.21230 0.00880 0.72220
C6+ C 0.28772 0.22272 0.77780
N'7+ N 0.29121 0.33917 0.87413
N'8+ N 0.37045 0.52083 0.89465
N'9+ N 0.41290 0.51430 0.81425
N'10+ N 0.36248 0.32820 0.73916

#END

data_2N2H5_BTO_0_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                 15.424
_cell_length_b                 4.808
_cell_length_c                 13.168
_cell_angle_alpha               90.00
_cell_angle_beta               124.11
_cell_angle_gamma                90.00
_cell_volume                   808.522
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.10682 -0.08401 0.55871
H*2 H -0.17460 -0.12583 0.47484
H*3 H -0.11796 -0.15636 0.62411
N4 N -0.09399 0.21494 0.57190
H*5 H -0.02719 0.25476 0.65592
H*6 H -0.08416 0.28547 0.50579
H*7 H -0.04607 -0.19361 0.56575
N1 N 0.40293 0.42377 0.06050
H*2 H 0.39285 0.32569 0.12261
H*3 H 0.46745 0.33447 0.06936
N4 N 0.42652 0.71348 0.09549
H*5 H 0.43757 0.80863 0.03421
H*6 H 0.36254 0.79980 0.08777
H*7 H 0.33819 0.38543 -0.02690
N'1+ N 0.07852 -0.37555 0.66085
N'2+ N 0.20922 -0.52949 0.83794
N'3+ N 0.12740 -0.35322 0.78170
N'4+ N 0.12715 -0.56698 0.63505
C5+ C 0.20755 -0.65919 0.74568
C6+ C 0.28343 -0.87307 0.76338
N'7+ N 0.28176 -1.00277 0.67112
N'8+ N 0.36358 -1.17904 0.72736
N'9+ N 0.41246 -1.15671 0.84821
N'10+ N 0.36383 -0.96528 0.87401

#END

data_2N2H5_BTO_0_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                 15.592
_cell_length_b                 4.908
_cell_length_c                 12.250
_cell_angle_alpha               90.00
_cell_angle_beta                85.25
_cell_angle_gamma                 90.00
_cell_volume                   934.218
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.41308 0.68191 0.60345
H*2 H -0.41027 0.58106 0.52963
H*3 H -0.47720 0.71397 0.62668
N4 N -0.37218 0.94489 0.58573
H*5 H -0.37609 1.04490 0.65912
H*6 H -0.30878 0.91123 0.56152
H*7 H -0.38767 0.55755 0.66067
N1 N 0.08323 -0.32748 0.85158
H*2 H 0.08335 -0.42717 0.77770
H*3 H 0.01980 -0.29332 0.87805
N4 N 0.12468 -0.06583 0.83243
H*5 H 0.12343 0.03306 0.90593
H*6 H 0.18734 -0.10155 0.80501
H*7 H 0.11002 -0.45381 0.90700
N'1+ N 0.08509 1.21624 0.08834
N'2+ N 0.21769 1.23718 0.01538
N'3+ N 0.13665 1.32568 0.00824
N'4+ N 0.13113 1.05344 0.14985
C5+ C 0.21275 1.06949 0.10333
C6+ C 0.28667 0.92331 0.14327
N'7+ N 0.28173 0.75562 0.23122
N'8+ N 0.36277 0.66712 0.23836
N'9+ N 0.41433 0.77656 0.15826
N'10+ N 0.36829 0.93935 0.09675

#END
```

S51. Optimized crystal structure coordinates for 5 polymorphs of **7d** (ionic form).

```
data_2GH_BTO_0_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
```

1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a 9.166
_cell_length_b 14.870
_cell_length_c 11.274
_cell_angle_alpha 90.00
_cell_angle_beta 41.39
_cell_angle_gamma 90.00
_cell_volume 1015.99
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.41603 0.16474 -0.01125
N2 N 0.48527 0.22897 0.02073
H*3 H 0.50269 0.21700 0.09784
H*4 H 0.52218 0.29136 -0.03127
N5 N 0.36835 0.08276 0.05933
H*6 H 0.31578 0.03326 0.03686
H*7 H 0.38348 0.06792 0.13719
N8 N 0.39448 0.18249 -0.11381
H*9 H 0.42961 0.24397 -0.16845
H*10 H 0.34243 0.13494 -0.13967
C1 C 0.08377 0.66477 0.01143
N2 N 0.13128 0.58279 -0.05911
H*3 H 0.11632 0.56803 -0.13711
H*4 H 0.18353 0.53322 -0.03648
N5 N 0.01495 0.72910 -0.02078
H*6 H -0.02183 0.79149 0.03119
H*7 H -0.00229 0.71720 -0.09803
N8 N 0.10508 0.68242 0.11418
H*9 H 0.15682 0.63480 0.14021
H*10 H 0.07007 0.74389 0.16879
N'1+ N 0.00862 0.07376 0.70349
N'2+ N 0.13709 0.11599 0.79751
N'3+ N 0.02487 0.14220 0.76892
N'4+ N 0.10979 0.00110 0.68767
C5+ C 0.18783 0.02871 0.74644
C6+ C 0.31195 -0.02879 0.75388
N'7+ N 0.36269 -0.11607 0.70281
N'8+ N 0.47491 -0.14228 0.73140
N'9+ N 0.49116 -0.07384 0.79683
N'10+ N 0.38999 -0.00118 0.81265

#END

data_2GH_BTO_0_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                   3.661
_cell_length_b                   19.220
_cell_length_c                   14.988
_cell_angle_alpha                 90.00
_cell_angle_beta                  83.04
_cell_angle_gamma                    90.00
_cell_volume                     1046.85
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.29184 0.16098 0.22990
N2 N 0.44425 0.22329 0.21083
H*3 H 0.41902 0.26234 0.25630
H*4 H 0.58912 0.23313 0.15039
N5 N 0.10158 0.14941 0.31045
H*6 H -0.01581 0.10273 0.32625
H*7 H 0.06962 0.18702 0.35788
N8 N 0.32969 0.11024 0.16842
H*9 H 0.47231 0.11787 0.10715
H*10 H 0.21678 0.06279 0.18143
C1 C 0.12866 0.58896 0.55642
N2 N 0.01909 0.60043 0.47576
H*3 H 0.03507 0.56280 0.42836
H*4 H -0.08289 0.64707 0.45986
N5 N 0.26254 0.52672 0.57563
H*6 H 0.34687 0.51694 0.63615
H*7 H 0.28329 0.48764 0.53018
N8 N 0.10435 0.63973 0.61787
H*9 H 0.00404 0.68714 0.60475
H*10 H 0.18558 0.63217 0.67922
N'1+ N 0.41121 0.47527 -0.74765
N'2+ N 0.33772 0.47216 -0.60080
N'3+ N 0.37416 0.51383 -0.67349
N'4+ N 0.39992 0.40742 -0.72530
C5+ C 0.35442 0.40674 -0.63437
C6+ C 0.32666 0.34304 -0.57909
N'7+ N 0.34336 0.27762 -0.61266
N'8+ N 0.30692 0.23595 -0.53997
N'9+ N 0.26987 0.27451 -0.46581
N'10+ N 0.28116 0.34236 -0.48816
```

```
#END

data_2GH_BTO_0_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                 3.558
_cell_length_b                 30.081
_cell_length_c                 9.810
_cell_angle_alpha               90.00
_cell_angle_beta                77.32
_cell_angle_gamma                90.00
_cell_volume                   1024.34
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.07523 -0.20701 0.29184
N2 N -0.15412 -0.21697 0.16823
H*3 H -0.25503 -0.24727 0.14964
H*4 H -0.11512 -0.19450 0.08981
N5 N -0.12960 -0.23741 0.39376
H*6 H -0.07184 -0.23058 0.48793
H*7 H -0.23003 -0.26810 0.37959
N8 N 0.05802 -0.16665 0.31352
H*9 H 0.10117 -0.14319 0.23795
H*10 H 0.11946 -0.15843 0.40612
C1 C -0.17705 0.45769 0.44217
N2 N -0.13633 0.48721 0.33801
H*3 H 0.01729 0.47990 0.24119
H*4 H -0.25799 0.51768 0.35308
N5 N -0.01283 0.41760 0.41922
H*6 H -0.03997 0.39481 0.49644
H*7 H 0.14322 0.40894 0.32399
N8 N -0.38200 0.46826 0.56928
H*9 H -0.50847 0.49836 0.58888
H*10 H -0.41638 0.44646 0.64944
N'1+ N 0.62170 0.65909 0.08820
N'2+ N 0.52478 0.68467 0.30161
N'3+ N 0.59154 0.69575 0.16550
N'4+ N 0.57542 0.62313 0.17183
C5+ C 0.51599 0.63971 0.30303
```

```
C6+ C 0.45023 0.61235 0.43085
N'7+ N 0.44144 0.56739 0.43227
N'8+ N 0.37468 0.55631 0.56838
N'9+ N 0.34452 0.59297 0.64568
N'10+ N 0.39080 0.62893 0.56205

#END

data_2GH_BTO_0_4
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P n a 21'
_symmetry_Int_Tables_number      33
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,1/2+z
3 1/2+x,1/2-y,z
4 -x,-y,1/2+z
_cell_length_a                 18.995
_cell_length_b                 3.668
_cell_length_c                 15.075
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma               90.00
_cell_volume                   1050.33
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.08844 -0.16773 0.40000
N2 N 0.02759 -0.01137 0.42333
H*3 H 0.01733 0.05442 0.48713
H*4 H -0.00991 0.04556 0.37783
N5 N 0.13713 -0.23997 0.46162
H*6 H 0.18346 -0.35798 0.44544
H*7 H 0.12902 -0.17866 0.52618
N8 N 0.10060 -0.25185 0.31505
H*9 H 0.06453 -0.19963 0.26743
H*10 H 0.14621 -0.37010 0.29599
C1 C 0.16280 0.46351 0.07074
N2 N 0.22659 0.60174 0.05407
H*3 H 0.23711 0.73158 -0.00356
H*4 H 0.26614 0.58041 0.09860
N5 N 0.11144 0.49576 0.01057
H*6 H 0.06286 0.39331 0.02183
H*7 H 0.11970 0.62351 -0.04790
N8 N 0.15037 0.29303 0.14758
H*9 H 0.18843 0.26564 0.19395
H*10 H 0.10256 0.18661 0.16152
```

N'1+ N 0.02475 -0.00179 0.60528
N'2+ N 0.02790 -0.08909 0.74865
N'3+ N -0.01414 -0.06205 0.67710
N'4+ N 0.09320 0.01209 0.62807
C5+ C 0.09389 -0.04247 0.71683
C6+ C 0.15817 -0.05013 0.77171
N'7+ N 0.22416 -0.00351 0.73989
N'8+ N 0.26620 -0.03055 0.81144
N'9+ N 0.22731 -0.09081 0.88326
N'10+ N 0.15886 -0.10469 0.86047

#END

data_2GH_BTO_0_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 3.742
_cell_length_b 20.584
_cell_length_c 13.860
_cell_angle_alpha 90.00
_cell_angle_beta 97.75
_cell_angle_gamma 90.00
_cell_volume 1057.82
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.13862 0.85246 0.33137
N2 N -0.17951 0.79168 0.29758
H*3 H -0.27869 0.75625 0.33690
H*4 H -0.11242 0.77941 0.23175
N5 N -0.22966 0.86732 0.41877
H*6 H -0.20096 0.91293 0.44568
H*7 H -0.32983 0.83336 0.46047
N8 N -0.00669 0.89838 0.27775
H*9 H 0.06379 0.88821 0.21152
H*10 H 0.02639 0.94460 0.30189
C1 C 0.54277 0.10244 0.19428
N2 N 0.53576 0.04166 0.22807
H*3 H 0.39732 0.00622 0.18877
H*4 H 0.66870 0.02940 0.29391
N5 N 0.36430 0.11728 0.10688

H*6 H 0.36603 0.16290 0.07997
H*7 H 0.22249 0.08332 0.06520
N8 N 0.72825 0.14837 0.24788
H*9 H 0.86497 0.13820 0.31410
H*10 H 0.73711 0.19459 0.22373
N'1+ N 0.03178 0.00580 0.40737
N'2+ N 0.10730 0.03932 0.55839
N'3+ N 0.07806 -0.01314 0.49990
N'4+ N 0.02961 0.07112 0.40305
C5+ C 0.07662 0.09076 0.49707
C6+ C 0.09238 0.15926 0.52857
N'7+ N 0.06170 0.21070 0.46725
N'8+ N 0.09094 0.26316 0.52574
N'9+ N 0.13722 0.24422 0.61827
N'10+ N 0.13939 0.17890 0.62259

#END

S52. Optimized crystal structure coordinates for 5 polymorphs of **7e** (ionic form).

data_2AGH_BTO_0_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 9.432
_cell_length_b 16.929
_cell_length_c 7.948
_cell_angle_alpha 84.56
_cell_angle_beta 31.01
_cell_angle_gamma 91.96
_cell_volume 634.169
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.06418 0.44860 -0.20618
N2 N 0.16907 0.45923 -0.35060
H*3 H 0.25583 0.41202 -0.39871
H*4 H 0.26477 0.51489 -0.41549
N5 N -0.18534 0.37340 -0.12352
H*6 H -0.09925 0.32573 -0.17116
N7 N -0.17819 0.51076 -0.14298
H*8 H -0.09344 0.56801 -0.20131
H*9 H -0.35479 0.49935 -0.03327
N10 N -0.42895 0.36268 0.02728
H*11 H -0.39344 0.34060 -0.11972
H*12 H -0.59309 0.32408 0.25994

C1 C 0.43598 -0.05142 0.29364
N2 N 0.66922 -0.04077 0.14925
H*3 H 0.75605 -0.08796 0.10105
H*4 H 0.76483 0.01489 0.08448
N5 N 0.31493 -0.12661 0.37615
H*6 H 0.40110 -0.17428 0.32841
N7 N 0.32187 0.01073 0.35697
H*8 H 0.40653 0.06798 0.29876
H*9 H 0.14529 -0.00069 0.46665
N10 N 0.07134 -0.13736 0.52692
H*11 H 0.10691 -0.15942 0.37984
H*12 H -0.09277 -0.17598 0.75952
N'1+ N -0.06828 0.11454 0.91855
N'2+ N 0.09502 0.24541 0.69224
N'3+ N -0.05233 0.17656 0.78416
N'4+ N 0.06825 0.14130 0.91786
C5+ C 0.16729 0.22220 0.77711
C6+ C 0.33243 0.27780 0.72325
N'7+ N 0.40470 0.25459 0.80812
N'8+ N 0.55205 0.32344 0.71620
N'9+ N 0.56800 0.38546 0.58181
N'10+ N 0.43147 0.35870 0.58250

#END

data_2AGH_BTO_0_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 9.298
_cell_length_b 10.512
_cell_length_c 12.204
_cell_angle_alpha 90.00
_cell_angle_beta 77.95
_cell_angle_gamma 90.00
_cell_volume 1166.54
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.13724 0.54265 0.89400
N2 N 0.22159 0.44751 0.91783
H*3 H 0.28432 0.45782 0.97561

H*4 H 0.22478 0.36266 0.87856
N5 N 0.13611 0.65430 0.94824
H*6 H 0.19886 0.66527 1.00637
N7 N 0.05474 0.52898 0.81794
H*8 H 0.05268 0.44674 0.77556
H*9 H -0.00707 0.60402 0.80311
N10 N 0.04778 0.75332 0.92299
H*11 H -0.02837 0.77824 0.99242
H*12 H 0.11099 0.82983 0.89282
C1 C 0.17242 0.16111 0.38276
N2 N 0.21530 0.06336 0.43873
H*3 H 0.28108 0.07661 0.49401
H*4 H 0.18294 -0.02648 0.42714
N5 N 0.21799 0.27944 0.40062
H*6 H 0.28407 0.29339 0.45603
N7 N 0.08585 0.14357 0.31003
H*8 H 0.04945 0.05630 0.29441
H*9 H 0.05666 0.22084 0.26992
N10 N 0.17284 0.38116 0.34191
H*11 H 0.11366 0.44470 0.39634
H*12 H 0.26175 0.42468 0.29353
N'1+ N 0.81360 -0.12417 0.09626
N'2+ N 0.92973 -0.02679 0.21028
N'3+ N 0.85418 -0.01127 0.12842
N'4+ N 0.86160 -0.21633 0.15628
C5+ C 0.93295 -0.15406 0.22609
C6+ C 1.00481 -0.21670 0.30863
N'7+ N 1.00803 -0.34397 0.32444
N'8+ N 1.08358 -0.35949 0.40630
N'9+ N 1.12416 -0.24659 0.43846
N'10+ N 1.07616 -0.15443 0.37844

#END

data_2AGH_BTO_0_3
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 11.981
_cell_length_b 12.411
_cell_length_c 9.419
_cell_angle_alpha 90.00
_cell_angle_beta 114.66
_cell_angle_gamma 90.00
_cell_volume 1272.84

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.16705 -0.06028 -0.16509
N2 N 0.20640 -0.11787 -0.25559
H*3 H 0.27562 -0.09144 -0.28124
H*4 H 0.16782 -0.18947 -0.30075
N5 N 0.22094 0.03480 -0.10716
H*6 H 0.29051 0.06180 -0.13249
N7 N 0.07596 -0.09513 -0.13140
H*8 H 0.03330 -0.16598 -0.17264
H*9 H 0.04975 -0.04838 -0.06235
N10 N 0.17944 0.09459 -0.01270
H*11 H 0.24857 0.10471 0.09562
H*12 H 0.14708 0.16750 -0.06252
C1 C 0.16721 -0.06023 0.33490
N2 N 0.20660 -0.11783 0.24445
H*3 H 0.27584 -0.09141 0.21884
H*4 H 0.16804 -0.18944 0.19928
N5 N 0.22109 0.03485 0.39283
H*6 H 0.29068 0.06184 0.36755
N7 N 0.07608 -0.09508 0.36853
H*8 H 0.03344 -0.16593 0.32729
H*9 H 0.04985 -0.04832 0.43755
N10 N 0.17954 0.09465 0.48724
H*11 H 0.24865 0.10478 0.59558
H*12 H 0.14720 0.16756 0.43740
N'1+ N 0.05134 0.28275 0.35478
N'2+ N -0.10165 0.39665 0.28025
N'3+ N -0.06529 0.29578 0.33087
N'4+ N 0.09415 0.37478 0.32041
C5+ C -0.00181 0.44392 0.27469
C6+ C 0.00195 0.55614 0.22525
N'7+ N 0.10179 0.60341 0.21969
N'8+ N 0.06543 0.70428 0.16907
N'9+ N -0.05120 0.71731 0.14516
N'10+ N -0.09401 0.62528 0.17953

#END

data_2AGH_BTO_0_4
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
```

3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 16.718
_cell_length_b 10.959
_cell_length_c 6.306
_cell_angle_alpha 90.00
_cell_angle_beta 88.16
_cell_angle_gamma 90.00
_cell_volume 1154.74
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.60614 0.15185 0.74815
N2 N 0.55558 0.24669 0.74661
H*3 H 0.49569 0.23427 0.74691
H*4 H 0.57603 0.33343 0.74511
N5 N 0.57645 0.03762 0.75013
H*6 H 0.51635 0.02452 0.75044
N7 N 0.68494 0.16830 0.74776
H*8 H 0.70943 0.25253 0.74630
H*9 H 0.72051 0.09336 0.74899
N10 N 0.62955 -0.06108 0.75174
H*11 H 0.61990 -0.11204 0.88519
H*12 H 0.62306 -0.11353 0.62006
C1 C -0.10650 -0.15178 0.75179
N2 N -0.05598 -0.24666 0.75343
H*3 H 0.00391 -0.23428 0.75319
H*4 H -0.07646 -0.33338 0.75497
N5 N -0.07678 -0.03758 0.74977
H*6 H -0.01668 -0.02452 0.74951
N7 N -0.18531 -0.16817 0.75211
H*8 H -0.20983 -0.25238 0.75361
H*9 H -0.22086 -0.09320 0.75081
N10 N -0.12985 0.06116 0.74805
H*11 H -0.12336 0.11363 0.87971
H*12 H -0.12016 0.11209 0.61457
N'1+ N 0.08348 0.55409 0.24973
N'2+ N 0.19771 0.65090 0.25414
N'3+ N 0.11765 0.66355 0.25361
N'4+ N 0.14034 0.46714 0.24762
C5+ C 0.21034 0.52897 0.25040
C6+ C 0.29000 0.47103 0.24948
N'7+ N 0.30263 0.34910 0.24574
N'8+ N 0.38269 0.33645 0.24627
N'9+ N 0.41686 0.44591 0.25015
N'10+ N 0.36000 0.53286 0.25226

#END

```
data_2AGH_BTO_0_5
_symmetry_cell_setting          orthorhombic
_symmetry_space_group_name_H-M   'P c a 21'
_symmetry_Int_Tables_number      29
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,y,1/2+z
3 1/2+x,-y,z
4 -x,-y,1/2+z
_cell_length_a                 6.303
_cell_length_b                 10.960
_cell_length_c                 16.719
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1154.96
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.50009 0.90183 0.59144
N2 N 0.50003 0.99668 0.64200
H*3 H 0.49998 0.98426 0.70189
H*4 H 0.50003 1.08340 0.62157
N5 N 0.50008 0.78761 0.62111
H*6 H 0.50003 0.77452 0.68120
N7 N 0.50015 0.91826 0.51265
H*8 H 0.50016 1.00248 0.48816
H*9 H 0.50020 0.84331 0.47706
N10 N 0.50015 0.68891 0.56800
H*11 H 0.63273 0.63721 0.57608
H*12 H 0.36758 0.63720 0.57605
C1 C 0.49995 -0.40182 0.30401
N2 N 0.49995 -0.49667 0.25345
H*3 H 0.49995 -0.48425 0.19356
H*4 H 0.49995 -0.58339 0.27388
N5 N 0.49995 -0.28760 0.27434
H*6 H 0.49995 -0.27451 0.21425
N7 N 0.49995 -0.41825 0.38281
H*8 H 0.49995 -0.50247 0.40729
H*9 H 0.49995 -0.34330 0.41839
N10 N 0.49995 -0.18890 0.32745
H*11 H 0.63252 -0.13719 0.31939
H*12 H 0.36738 -0.13719 0.31939
N'1+ N -0.00005 0.08647 0.81525
N'2+ N 0.00004 0.28289 0.83788
N'3+ N 0.00002 0.19594 0.78104
N'4+ N -0.00008 0.09910 0.89532
```

C5+ C -0.00003 0.22104 0.90791
C6+ C -0.00003 0.27896 0.98755
N'7+ N -0.00010 0.21711 1.05758
N'8+ N -0.00008 0.30406 1.11442
N'9+ N -0.00001 0.41353 1.08021
N'10+ N 0.00002 0.40090 1.00014

#END

S53. Optimized crystal structure coordinates for 5 polymorphs of **7f** (ionic form).

data_2DAGH_BTO_0_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 14.637
_cell_length_b 7.407
_cell_length_c 12.806
_cell_angle_alpha 90.00
_cell_angle_beta 80.20
_cell_angle_gamma 90.00
_cell_volume 1368.12
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.18994 0.43729 -0.04173
N2 N -0.23429 0.33037 0.03480
H*3 H -0.26906 0.39060 0.10119
N4 N -0.19321 0.61769 -0.02775
H*5 H -0.15983 0.69977 -0.08529
N6 N -0.14322 0.36585 -0.13051
H*7 H -0.14265 0.22949 -0.13759
H*8 H -0.10919 0.44329 -0.18944
N9 N -0.24296 0.68812 0.06653
N10 N -0.23064 0.14290 0.01982
H*11 H -0.29586 0.09329 0.02223
H*12 H -0.20001 0.75900 0.10612
H*13 H -0.29531 0.76877 0.05085
H*14 H -0.20078 0.08354 0.07737
C1 C 0.09033 0.06276 0.39747
N2 N 0.13467 0.16964 0.32092
H*3 H 0.16944 0.10938 0.25454
N4 N 0.09358 -0.11765 0.38352
H*5 H 0.06020 -0.19971 0.44107

N6 N 0.04362 0.13423 0.48625
H*7 H 0.04306 0.27060 0.49331
H*8 H 0.00958 0.05681 0.54519
N9 N 0.14332 -0.18812 0.28924
N10 N 0.13104 0.35711 0.33589
H*11 H 0.10118 0.41646 0.27833
H*12 H 0.19566 -0.26878 0.30492
H*13 H 0.10035 -0.25901 0.24966
H*14 H 0.19626 0.40671 0.33346
N'1+ N 0.34123 -0.57069 0.19302
N'2+ N 0.34611 -0.31482 0.27693
N'3+ N 0.30072 -0.47245 0.27482
N'4+ N 0.41411 -0.47975 0.13961
C5+ C 0.41579 -0.32228 0.19279
C6+ C 0.48459 -0.17770 0.16295
N'7+ N 0.55427 -0.18516 0.07881
N'8+ N 0.59966 -0.02753 0.08092
N'9+ N 0.55915 0.07071 0.16272
N'10+ N 0.48627 -0.02023 0.21613

#END

data_2DAGH_BTO_0_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 16.661
_cell_length_b 14.446
_cell_length_c 6.487
_cell_angle_alpha 90.00
_cell_angle_beta 121.45
_cell_angle_gamma 90.00
_cell_volume 1331.96
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.09247 0.77724 -0.54735
N2 N -0.15166 0.84786 -0.59438
H*3 H -0.12411 0.91279 -0.55443
N4 N -0.00017 0.79493 -0.45042
H*5 H 0.04521 0.74188 -0.41417
N6 N -0.12463 0.69063 -0.59597

H*7 H -0.19458 0.68059 -0.66881
H*8 H -0.08157 0.63614 -0.56234
N9 N 0.03117 0.88678 -0.40166
N10 N -0.24756 0.82904 -0.69516
H*11 H -0.28582 0.86112 -0.85830
H*12 H 0.07821 0.89530 -0.22181
H*13 H 0.06102 0.90475 -0.49859
H*14 H -0.26867 0.85169 -0.58217
C1 C 0.59247 0.22275 0.04734
N2 N 0.65164 0.15211 0.09432
H*3 H 0.62406 0.08720 0.05430
N4 N 0.50016 0.20509 -0.04964
H*5 H 0.45480 0.25815 -0.08586
N6 N 0.62466 0.30935 0.09605
H*7 H 0.69462 0.31937 0.16892
H*8 H 0.58162 0.36385 0.06245
N9 N 0.46879 0.11325 -0.09850
N10 N 0.74754 0.17090 0.19515
H*11 H 0.76866 0.14826 0.08216
H*12 H 0.43892 0.09528 -0.00160
H*13 H 0.42175 0.10475 -0.27836
H*14 H 0.78579 0.13881 0.35827
N'1+ N -0.38310 -0.14076 0.66971
N'2+ N -0.32729 -0.01319 0.87815
N'3+ N -0.38770 -0.08389 0.82429
N'4+ N -0.31957 -0.10867 0.61862
C5+ C -0.28604 -0.02992 0.74922
C6+ C -0.21394 0.02988 0.75084
N'7+ N -0.17269 0.01315 0.62191
N'8+ N -0.11228 0.08385 0.67577
N'9+ N -0.11688 0.14072 0.83035
N'10+ N -0.18041 0.10863 0.88144

#END

data_2DAGH_BTO_0_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 17.179
_cell_length_b 6.844
_cell_length_c 12.671
_cell_angle_alpha 90.00
_cell_angle_beta 70.26
_cell_angle_gamma 90.00

```
_cell_volume                    1402.22
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25027 0.30150 0.53378
N2 N 0.16785 0.30142 0.58163
H*3 H 0.14412 0.31495 0.66643
N4 N 0.29763 0.31926 0.59910
H*5 H 0.36013 0.31947 0.56361
N6 N 0.28486 0.28422 0.42295
H*7 H 0.24683 0.27123 0.37713
H*8 H 0.34680 0.28384 0.38473
N9 N 0.25920 0.33713 0.71526
N10 N 0.11893 0.28292 0.51329
H*11 H 0.08218 0.40282 0.52197
H*12 H 0.27572 0.22399 0.75542
H*13 H 0.27467 0.46667 0.74239
H*14 H 0.08324 0.16071 0.53496
C1 C -0.00609 0.25395 0.97216
N2 N 0.07577 0.28150 0.92926
H*3 H 0.10065 0.30966 0.84577
N4 N -0.05143 0.26454 0.90385
H*5 H -0.11349 0.24387 0.93559
N6 N -0.04211 0.21655 1.08105
H*7 H -0.00558 0.20993 1.12927
H*8 H -0.10367 0.19519 1.11556
N9 N -0.01154 0.30411 0.78985
N10 N 0.12259 0.27031 1.00070
H*11 H 0.15167 0.40003 1.00059
H*12 H -0.01983 0.19143 0.74227
H*13 H -0.03345 0.43054 0.76809
H*14 H 0.16526 0.16148 0.97483
N'1+ N 0.44987 0.31388 0.34624
N'2+ N 0.56785 0.45333 0.32987
N'3+ N 0.48504 0.47207 0.37124
N'4+ N 0.50881 0.18775 0.28789
C5+ C 0.58110 0.27683 0.27879
C6+ C 0.66354 0.19255 0.22079
N'7+ N 0.67679 0.01605 0.16971
N'8+ N 0.75960 -0.00269 0.12834
N'9+ N 0.79477 0.15550 0.15334
N'10+ N 0.73583 0.28163 0.21169

#END

data_2DAGH_BTO_0_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                14.467
_cell_length_b                7.440
_cell_length_c                27.348
_cell_angle_alpha              90.00
_cell_angle_beta               111.07
_cell_angle_gamma               90.00
_cell_volume                  2746.79
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.37518 0.12470 0.73359
N2 N 0.38219 0.01388 0.69650
H*3 H 0.38458 0.07005 0.66309
N4 N 0.37165 0.30352 0.72519
H*5 H 0.36635 0.38854 0.75305
N6 N 0.37176 0.05865 0.77819
H*7 H 0.37462 -0.07671 0.78281
H*8 H 0.36648 0.13913 0.80679
N9 N 0.37542 0.36825 0.67786
N10 N 0.38582 -0.17191 0.70546
H*11 H 0.45042 -0.22290 0.70441
H*12 H 0.31260 0.43802 0.65791
H*13 H 0.43598 0.44799 0.68473
H*14 H 0.32732 -0.23285 0.67766
C1 C 0.12238 0.25969 0.48644
N2 N 0.12110 0.34757 0.44348
H*3 H 0.12305 0.27299 0.41272
N4 N 0.12614 0.07865 0.48709
H*5 H 0.12714 0.01090 0.51946
N6 N 0.11996 0.35044 0.52797
H*7 H 0.11716 0.48649 0.52573
H*8 H 0.12085 0.28759 0.56084
N9 N 0.12861 -0.01237 0.44276
N10 N 0.11719 0.53580 0.44304
H*11 H 0.05478 0.57843 0.41376
H*12 H 0.19206 -0.08557 0.45192
H*13 H 0.06846 -0.09403 0.42803
H*14 H 0.17809 0.58687 0.43759
```

```
N'1+ N 0.53023 -0.76471 0.13420
N'2+ N 0.57426 -0.51027 0.17610
N'3+ N 0.52903 -0.66909 0.17502
N'4+ N 0.57627 -0.67081 0.10757
C5+ C 0.60280 -0.51428 0.13412
C6+ C 0.65590 -0.36728 0.11926
N'7+ N 0.68444 -0.37129 0.07728
N'8+ N 0.72967 -0.21247 0.07836
N'9+ N 0.72847 -0.11685 0.11918
N'10+ N 0.68243 -0.21075 0.14581

#END

data_2DAGH_BTO_0_5
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P 1'
_symmetry_Int_Tables_number      1
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
_cell_length_a                  9.465
_cell_length_b                  6.995
_cell_length_c                  7.437
_cell_angle_alpha                95.33
_cell_angle_beta                 66.08
_cell_angle_gamma                130.36
_cell_volume                    332.638
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.09144 0.42793 0.39356
N2 N -0.17879 0.50731 0.36540
H*3 H -0.24763 0.54999 0.48455
N4 N -0.09834 0.40820 0.57605
H*5 H -0.03260 0.34822 0.59881
N6 N 0.00103 0.36930 0.24277
H*7 H 0.00250 0.38699 0.10811
H*8 H 0.06807 0.30901 0.25987
N9 N -0.19680 0.47139 0.73108
N10 N -0.17112 0.52745 0.17533
H*11 H -0.09353 0.71346 0.11505
H*12 H -0.31889 0.31485 0.85097
H*13 H -0.09362 0.62107 0.77596
H*14 H -0.31828 0.40795 0.18989
C1 C 0.44264 0.83325 -0.37702
N2 N 0.52999 0.75387 -0.34886
H*3 H 0.59883 0.71119 -0.46801
N4 N 0.44954 0.85298 -0.55951
```

H*5 H 0.38380 0.91296 -0.58227
N6 N 0.35017 0.89188 -0.22623
H*7 H 0.34870 0.87419 -0.09157
H*8 H 0.28313 0.95217 -0.24333
N9 N 0.54800 0.78979 -0.71454
N10 N 0.52232 0.73373 -0.15879
H*11 H 0.66948 0.85323 -0.17335
H*12 H 0.44482 0.64011 -0.75942
H*13 H 0.67009 0.94633 -0.83443
H*14 H 0.44473 0.54772 -0.09851
N'1+ N -0.01621 -0.02802 0.93882
N'2+ N -0.00797 0.15542 0.70776
N'3+ N -0.08783 0.07179 0.90818
N'4+ N 0.11226 -0.01216 0.75920
C5+ C 0.11501 0.10165 0.61880
C6+ C 0.23619 0.15953 0.39774
N'7+ N 0.35917 0.10576 0.30878
N'8+ N 0.43903 0.18939 0.10836
N'9+ N 0.36741 0.28920 0.07772
N'10+ N 0.23894 0.27334 0.25734

#END

S54. Optimized crystal structure coordinates for 5 polymorphs of **7g** (ionic form).

data_2TAGH_BTO_0_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 3.949
_cell_length_b 12.776
_cell_length_c 17.918
_cell_angle_alpha 97.21
_cell_angle_beta 62.60
_cell_angle_gamma 106.36
_cell_volume 770.086
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.66063 0.26974 0.55980
N2 N 0.82873 0.25462 0.47641
H*3 H 0.81216 0.17657 0.45528
N4 N 0.67400 0.37103 0.59100
H*5 H 0.81432 0.43417 0.54935
N6 N 0.47917 0.18357 0.61199
H*7 H 0.35541 0.19848 0.67477

N8 N 0.49606 0.38466 0.67839
N9 N 1.01657 0.34603 0.42321
H*10 H 0.88494 0.34307 0.38540
H*11 H 0.70142 0.42880 0.69726
H*12 H 0.27959 0.42383 0.69540
H*13 H 1.30678 0.34804 0.38727
N14 N 0.46926 0.07853 0.57780
H*15 H 0.60644 0.03983 0.59766
H*16 H 0.18461 0.03487 0.59580
C1 C 0.16138 0.76979 0.05981
N2 N 0.17457 0.87107 0.09104
H*3 H 0.31397 0.93422 0.04941
N4 N -0.01888 0.68360 0.11197
H*5 H -0.14189 0.69849 0.17476
N6 N 0.32845 0.75470 -0.02358
H*7 H 0.31206 0.67667 -0.04475
N8 N -0.02863 0.57859 0.07776
N9 N -0.00228 0.88465 0.17844
H*10 H -0.21923 0.92371 0.19565
H*11 H 0.10952 0.53999 0.09742
H*12 H -0.31327 0.53480 0.09592
H*13 H 0.20356 0.92890 0.19715
N14 N 0.51505 0.84613 -0.07676
H*15 H 0.80524 0.84827 -0.11289
H*16 H 0.38246 0.84307 -0.11439
N'1+ N 0.46290 0.01887 0.25156
N'2+ N 0.44331 0.15303 0.34087
N'3+ N 0.32646 0.04441 0.33263
N'4+ N 0.67237 0.11015 0.20476
C5+ C 0.65630 0.19191 0.26118
C6+ C 0.84610 0.30819 0.23874
N'7+ N 1.05909 0.34707 0.15905
N'8+ N 1.17594 0.45569 0.16729
N'9+ N 1.03950 0.48123 0.24836
N'10+ N 0.83003 0.38995 0.29516

#END

data_2TAGH_BTO_0_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z

8 1/2+x,1/2-y,1/2+z
_cell_length_a 19.897
_cell_length_b 7.910
_cell_length_c 20.282
_cell_angle_alpha 90.00
_cell_angle_beta 105.01
_cell_angle_gamma 90.00
_cell_volume 3083.18
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.14511 0.53531 -0.33495
N2 N -0.21453 0.55180 -0.35204
H*3 H -0.23849 0.55847 -0.31352
N4 N -0.11095 0.52594 -0.38378
H*5 H -0.13957 0.53181 -0.43314
N6 N -0.10985 0.52819 -0.26903
H*7 H -0.05728 0.51566 -0.25819
N8 N -0.03838 0.50873 -0.36459
N9 N -0.25018 0.55894 -0.42131
H*10 H -0.27614 0.67076 -0.43173
H*11 H -0.02436 0.39916 -0.38381
H*12 H -0.01594 0.60863 -0.38237
H*13 H -0.28456 0.46129 -0.43317
N14 N -0.14677 0.53826 -0.21896
H*15 H -0.13904 0.43128 -0.19003
H*16 H -0.13062 0.64075 -0.18859
C1 C 0.14511 -0.03529 0.33496
N2 N 0.21453 -0.05178 0.35205
H*3 H 0.23849 -0.05847 0.31353
N4 N 0.11095 -0.02589 0.38379
H*5 H 0.13957 -0.03174 0.43315
N6 N 0.10985 -0.02820 0.26903
H*7 H 0.05728 -0.01566 0.25820
N8 N 0.03838 -0.00868 0.36460
N9 N 0.25018 -0.05889 0.42132
H*10 H 0.28456 0.03876 0.43318
H*11 H 0.01594 -0.10857 0.38238
H*12 H 0.02436 0.10090 0.38381
H*13 H 0.27614 -0.17071 0.43175
N14 N 0.14677 -0.03829 0.21897
H*15 H 0.13062 -0.14079 0.18861
H*16 H 0.13904 0.06868 0.19003
N'1+ N -0.11548 0.78956 -0.11608
N'2+ N -0.09296 0.80149 -0.00483
N'3+ N -0.14279 0.81660 -0.06374
N'4+ N -0.04711 0.75609 -0.09270
C5+ C -0.03437 0.76413 -0.02393
C6+ C 0.03437 0.73587 0.02393

```
N'7+ N 0.09296 0.69851 0.00483
N'8+ N 0.14279 0.68340 0.06374
N'9+ N 0.11548 0.71044 0.11608
N'10+ N 0.04711 0.74391 0.09270

#END

data_2TAGH_BTO_0_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                  20.097
_cell_length_b                  10.781
_cell_length_c                  3.946
_cell_angle_alpha                 68.48
_cell_angle_beta                 90.36
_cell_angle_gamma                   76.65
_cell_volume                    769.951
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.08537 -0.21000 -0.79161
N2 N -0.10216 -0.07193 -0.93189
H*3 H -0.06314 -0.02411 -0.97883
N4 N -0.13485 -0.27817 -0.72446
H*5 H -0.18446 -0.22141 -0.78369
N6 N -0.01910 -0.27991 -0.71847
H*7 H -0.00851 -0.38448 -0.61231
N8 N -0.11596 -0.42249 -0.57779
N9 N -0.17180 -0.00127 -1.00591
H*10 H -0.18277 0.05838 -1.27760
H*11 H -0.13482 -0.45849 -0.33111
H*12 H -0.13466 -0.45917 -0.75231
H*13 H -0.18293 0.05906 -0.85640
N14 N 0.03165 -0.20625 -0.79113
H*15 H 0.06140 -0.22955 -0.55552
H*16 H 0.06156 -0.23023 -0.97672
C1 C 0.58538 0.21003 0.79233
N2 N 0.60219 0.07196 0.93273
H*3 H 0.56319 0.02411 0.97848
N4 N 0.63485 0.27824 0.72670
H*5 H 0.68446 0.22151 0.78714
N6 N 0.51910 0.27989 0.71756
H*7 H 0.50850 0.38447 0.61137
```

N8 N 0.61593 0.42256 0.57987
N9 N 0.67184 0.00134 1.00847
H*10 H 0.68320 -0.05902 0.85915
H*11 H 0.63439 0.45930 0.75494
H*12 H 0.63501 0.45854 0.33384
H*13 H 0.68258 -0.05827 1.28026
N14 N 0.46837 0.20619 0.78866
H*15 H 0.43823 0.23019 0.97345
H*16 H 0.43886 0.22943 0.55234
N'1+ N 0.13539 0.73432 -0.22755
N'2+ N 0.24762 0.68770 -0.18196
N'3+ N 0.18922 0.78891 -0.27978
N'4+ N 0.15726 0.59605 -0.09427
C5+ C 0.22666 0.56962 -0.06838
C6+ C 0.27336 0.43032 0.06604
N'7+ N 0.25240 0.31224 0.17962
N'8+ N 0.31080 0.21103 0.27744
N'9+ N 0.36463 0.26562 0.22521
N'10+ N 0.34276 0.40389 0.09193

#END

data_2TAGH_BTO_0_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 20.012
_cell_length_b 7.897
_cell_length_c 20.141
_cell_angle_alpha 90.00
_cell_angle_beta 104.63
_cell_angle_gamma 90.00
_cell_volume 3079.78
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.35495 0.51543 0.66468
N2 N 0.28582 0.52464 0.64778

H*3 H 0.26186 0.52802 0.68665
N4 N 0.38911 0.51064 0.61539
H*5 H 0.36071 0.51426 0.56583
N6 N 0.38992 0.51100 0.73088
H*7 H 0.44228 0.50402 0.74155
N8 N 0.46136 0.50102 0.63439
N9 N 0.25047 0.52910 0.57822
H*10 H 0.22277 0.63834 0.56765
H*11 H 0.47724 0.39325 0.61518
H*12 H 0.48190 0.60375 0.61621
H*13 H 0.21811 0.42784 0.56662
N14 N 0.35302 0.51616 0.78143
H*15 H 0.36251 0.40945 0.81069
H*16 H 0.36717 0.61994 0.81173
C1 C 0.64494 -0.01548 0.33528
N2 N 0.71407 -0.02466 0.35219
H*3 H 0.73804 -0.02801 0.31332
N4 N 0.61077 -0.01074 0.38457
H*5 H 0.63916 -0.01435 0.43412
N6 N 0.60998 -0.01104 0.26908
H*7 H 0.55762 -0.00408 0.25840
N8 N 0.53851 -0.00114 0.36555
N9 N 0.74941 -0.02914 0.42175
H*10 H 0.78177 0.07214 0.43337
H*11 H 0.51798 -0.10389 0.38372
H*12 H 0.52263 0.10661 0.38477
H*13 H 0.77712 -0.13836 0.43232
N14 N 0.64690 -0.01616 0.21854
H*15 H 0.63275 -0.11993 0.18823
H*16 H 0.63740 0.09056 0.18928
N'1+ N -0.11686 0.76661 -0.11507
N'2+ N -0.09366 0.77718 -0.00313
N'3+ N -0.14412 0.78296 -0.06168
N'4+ N -0.04790 0.74973 -0.09276
C5+ C -0.03474 0.75662 -0.02354
C6+ C 0.03472 0.74344 0.02350
N'7+ N 0.09364 0.72288 0.00309
N'8+ N 0.14410 0.71710 0.06164
N'9+ N 0.11684 0.73345 0.11503
N'10+ N 0.04788 0.75033 0.09272

#END

data_2TAGH_BTO_0_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                10.047
_cell_length_b                3.946
_cell_length_c                20.447
_cell_angle_alpha              78.83
_cell_angle_beta               75.69
_cell_angle_gamma                89.61
_cell_volume                  769.88
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.17076 0.60700 0.39500
N2 N -0.20436 0.53888 0.46403
H*3 H -0.12633 0.51142 0.48795
N4 N -0.26972 0.64563 0.36090
H*5 H -0.36894 0.62132 0.38927
N6 N -0.03820 0.63649 0.36006
H*7 H -0.01701 0.68827 0.30778
N8 N -0.23191 0.71671 0.28875
N9 N -0.34365 0.50930 0.49935
H*10 H -0.36488 0.69102 0.52926
H*11 H -0.27034 0.52566 0.27065
H*12 H -0.26859 0.94763 0.27049
H*13 H -0.36663 0.26905 0.52941
N14 N 0.06328 0.59499 0.39691
H*15 H 0.12206 0.39334 0.38517
H*16 H 0.12382 0.81531 0.38501
C1 C 0.17075 0.89301 0.10500
N2 N 0.26971 0.85436 0.13910
H*3 H 0.36893 0.87871 0.11073
N4 N 0.03819 0.86347 0.13994
H*5 H 0.01700 0.81165 0.19222
N6 N 0.20435 0.96120 0.03597
H*7 H 0.12632 0.98868 0.01205
N8 N -0.06329 0.90500 0.10309
N9 N 0.23190 0.78320 0.21125
H*10 H 0.27032 0.97423 0.22936
H*11 H -0.12382 0.68467 0.11498
H*12 H -0.12208 1.10663 0.11484
H*13 H 0.26858 0.55228 0.22950
N14 N 0.34364 0.99083 0.00065
H*15 H 0.36488 0.80915 -0.02927
H*16 H 0.36662 1.23110 -0.02941
N'1+ N 0.37843 -0.40330 0.89447
N'2+ N 0.31455 -0.30723 0.79802
N'3+ N 0.27081 -0.37998 0.86716
N'4+ N 0.49522 -0.34638 0.84387
C5+ C 0.45332 -0.28768 0.78482
C6+ C 0.54670 -0.21226 0.71518
N'7+ N 0.68547 -0.19271 0.70198
```

N'8+ N 0.72921 -0.11996 0.63284
N'9+ N 0.62159 -0.09664 0.60553
N'10+ N 0.50480 -0.15356 0.65613

#END

S55. Optimized crystal structure coordinates for 5 polymorphs of **8a** (ionic form).

data_2NH4_BTO_1_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 19.891
_cell_length_b 11.682
_cell_length_c 4.019
_cell_angle_alpha 90.00
_cell_angle_beta 50.07
_cell_angle_gamma 90.00
_cell_volume 716.128
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.86733 0.44944 0.23889
H*2 H 0.89694 0.52445 0.07242
H*3 H 0.83213 0.41636 0.15496
H*4 H 0.91442 0.39158 0.16136
H*5 H 0.82583 0.46537 0.56681
N1 N 0.13533 -0.05252 0.82586
H*2 H 0.10244 0.01594 1.03146
H*3 H 0.16008 -0.10276 0.93501
H*4 H 0.09289 -0.10000 0.81779
H*5 H 0.18592 -0.02326 0.51918
N'1+ N 0.23506 0.66799 -0.10247
N2+ N 0.28667 0.82460 -0.06217
N'3+ N 0.22268 0.78013 -0.05500
N'4+ N 0.30460 0.63800 -0.14014
C5+ C 0.33773 0.73553 -0.11542
C6+ C 0.41468 0.74118 -0.14229
N'7+ N 0.45997 0.64625 -0.19560
N'8+ N 0.52458 0.68537 -0.20504
N'9+ N 0.51869 0.79863 -0.15960
N'10+ N 0.44993 0.83663 -0.11916
O11+ O 0.29253 0.93333 -0.02288

```
#END

data_2NH4_BTO_1_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                 9.933
_cell_length_b                 11.716
_cell_length_c                 8.061
_cell_angle_alpha               90.00
_cell_angle_beta                129.68
_cell_angle_gamma               90.00
_cell_volume                   721.982
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.22570 0.03609 0.12455
H*2 H 0.13350 0.01231 -0.03411
H*3 H 0.16523 0.07647 0.17457
H*4 H 0.29000 -0.03517 0.21771
H*5 H 0.31407 0.09076 0.14002
N1 N 0.24056 0.06504 0.65009
H*2 H 0.30318 -0.00365 0.75193
H*3 H 0.17565 0.11001 0.68956
H*4 H 0.33105 0.11715 0.66511
H*5 H 0.15236 0.03665 0.49376
N'1+ N -0.04133 0.66966 0.29519
N2+ N 0.07722 0.82473 0.29917
N'3+ N -0.05511 0.78227 0.28893
N'4+ N 0.09480 0.63745 0.30909
C5+ C 0.17061 0.73399 0.31175
C6+ C 0.32505 0.73721 0.32576
N'7+ N 0.40633 0.64079 0.33748
N'8+ N 0.53938 0.67788 0.34802
N'9+ N 0.53869 0.79140 0.34292
N'10+ N 0.40490 0.83160 0.32888
O11+ O 0.09959 0.93335 0.29639

#END

data_2NH4_BTO_1_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                   19.890
_cell_length_b                   11.683
_cell_length_c                   4.020
_cell_angle_alpha                 90.00
_cell_angle_beta                  129.89
_cell_angle_gamma                    90.00
_cell_volume                     716.75
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.13245 -0.05056 0.76262
H*2 H -0.10276 0.02434 0.92954
H*3 H -0.17391 -0.03444 0.43507
H*4 H -0.08547 -0.10848 0.83941
H*5 H -0.16766 -0.08367 0.84646
N1 N -0.13559 0.55242 -0.17648
H*2 H -0.09311 0.59995 -0.18410
H*3 H -0.10275 0.48396 0.02896
H*4 H -0.16044 0.60261 -0.06773
H*5 H -0.18606 0.52316 -0.48305
N'1+ N 0.23498 0.16802 0.10205
N2+ N 0.28675 0.32463 0.06296
N'3+ N 0.22272 0.28018 0.05551
N'4+ N 0.30447 0.13801 0.13939
C5+ C 0.33771 0.23554 0.11542
C6+ C 0.41465 0.24118 0.14223
N'7+ N 0.45983 0.14623 0.19471
N'8+ N 0.52448 0.18533 0.20438
N'9+ N 0.51870 0.29861 0.15986
N'10+ N 0.45000 0.33663 0.11983
O11+ O 0.29273 0.43338 0.02455

#END

data_2NH4_BTO_1_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                 10.022
_cell_length_b                 7.492
_cell_length_c                 7.240
_cell_angle_alpha               66.36
_cell_angle_beta               124.93
_cell_angle_gamma               82.35
_cell_volume                   357.513
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.11941 0.14128 -0.06442
H*2 H 0.05189 0.21269 -0.02627
H*3 H 0.22587 0.17728 -0.01524
H*4 H 0.17261 -0.02827 0.05523
H*5 H 0.02727 0.20342 -0.27140
N1 N 0.35502 0.34143 0.51830
H*2 H 0.42371 0.26712 0.48350
H*3 H 0.30927 0.50959 0.40568
H*4 H 0.24321 0.31450 0.45735
H*5 H 0.44389 0.27451 0.72667
N'1+ N 0.43057 0.19652 0.12420
N2+ N 0.65485 0.23140 0.40800
N'3+ N 0.50358 0.20811 0.33718
N'4+ N 0.52862 0.21137 0.05414
C5+ C 0.67006 0.23337 0.23068
C6+ C 0.81145 0.25499 0.22607
N'7+ N 0.81146 0.25461 0.03890
N'8+ N 0.95931 0.27735 0.09955
N'9+ N 1.04478 0.29086 0.31334
N'10+ N 0.95489 0.27728 0.39829
O11+ O 0.75735 0.24749 0.61096

#END

data_2NH4_BTO_1_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                 17.903
_cell_length_b                 7.333
_cell_length_c                 7.633
```

```
_cell_angle_alpha                149.47
_cell_angle_beta                 68.87
_cell_angle_gamma                128.49
_cell_volume                     357.473
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.39892 0.55057 0.42960
H*2 H 0.34489 0.21955 0.14481
H*3 H 0.39347 0.78257 0.56793
H*4 H 0.38288 0.52662 0.55489
H*5 H 0.47445 0.67355 0.45078
N1 N 0.12057 0.98909 0.07585
H*2 H 0.11205 0.72677 -0.06667
H*3 H 0.18316 1.31654 0.34536
H*4 H 0.13512 0.97822 -0.07532
H*5 H 0.05194 0.93484 0.10004
N'1+ N 0.06310 0.16570 0.82604
N2+ N 0.19584 0.40965 0.75244
N'3+ N 0.10844 0.36493 0.79931
N'4+ N 0.11770 0.07947 0.79832
C5+ C 0.20137 0.23089 0.75196
C6+ C 0.28181 0.20234 0.70977
N'7+ N 0.27850 0.01637 0.71407
N'8+ N 0.36377 0.05157 0.66845
N'9+ N 0.41623 0.24950 0.63797
N'10+ N 0.36654 0.34914 0.66291
O11+ O 0.25780 0.59393 0.71711

#END
```

S56. Optimized crystal structure coordinates for 5 polymorphs of **8b** (ionic form).

```
data_2NH3OH_BTO_1_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                   18.260
_cell_length_b                   12.183
_cell_length_c                   7.440
```

```
_cell_angle_alpha                90.00
_cell_angle_beta                 90.00
_cell_angle_gamma                90.00
_cell_volume                   1655.11
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.11271 0.54715 0.47725
H*2 H -0.07137 0.50962 0.40571
H*3 H -0.13858 0.48898 0.55581
H*4 H -0.09028 0.60831 0.55610
O5 O -0.15979 0.59008 0.34526
H*6 H -0.20001 0.62659 0.40781
N1 N 0.60493 0.02181 -0.04438
H*2 H 0.56557 -0.00961 -0.12930
H*3 H 0.58022 0.07527 0.04469
H*4 H 0.62965 -0.04229 0.02330
O5 O 0.65435 0.07624 -0.15862
H*6 H 0.69279 0.10742 -0.08297
N'1+ N -0.03054 0.67538 0.15904
N2+ N 0.02374 0.82423 0.24071
N'3+ N -0.03713 0.78360 0.15975
N'4+ N 0.03225 0.64424 0.23641
C5+ C 0.06697 0.73691 0.28844
C6+ C 0.13812 0.73979 0.37932
N'7+ N 0.17578 0.64703 0.41949
N'8+ N 0.23701 0.68249 0.50047
N'9+ N 0.23644 0.79158 0.50892
N'10+ N 0.17471 0.83039 0.43355
O11+ O 0.03381 0.92857 0.26232

#END

data_2NH3OH_BTO_1_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                 10.492
_cell_length_b                 9.939
_cell_length_c                 8.041
_cell_angle_alpha                90.00
_cell_angle_beta                 106.23
```

```
_cell_angle_gamma              90.00
_cell_volume                  805.098
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.40209 0.46273 0.76953
H*2 H 0.33114 0.46723 0.65147
H*3 H 0.38061 0.53447 0.85067
H*4 H 0.40146 0.36745 0.82062
O5 O 0.52236 0.49025 0.73145
H*6 H 0.59268 0.48695 0.84060
N1 N 0.44987 0.21932 0.31424
H*2 H 0.34757 0.21790 0.27572
H*3 H 0.48432 0.12144 0.32491
H*4 H 0.48305 0.27177 0.22352
O5 O 0.48305 0.28512 0.47543
H*6 H 0.57982 0.28862 0.51678
N'1+ N -0.25779 0.55877 -0.02748
N2+ N -0.10417 0.70691 -0.00612
N'3+ N -0.22908 0.67132 -0.09740
N'4+ N -0.15635 0.51998 0.10561
C5+ C -0.05904 0.61211 0.12062
C6+ C 0.07022 0.60761 0.25108
N'7+ N 0.10328 0.50777 0.37040
N'8+ N 0.22688 0.53798 0.46507
N'9+ N 0.26676 0.65079 0.40586
N'10+ N 0.17011 0.69740 0.27065
O11+ O -0.04690 0.81370 -0.04307

#END

data_2NH3OH_BTO_1_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                 7.983
_cell_length_b                 7.567
_cell_length_c                 7.981
_cell_angle_alpha               77.69
_cell_angle_beta               122.64
_cell_angle_gamma               85.97
_cell_volume                  386.452
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.32050 0.17287 0.26259
H*2 H -0.41224 0.08771 0.27202
H*3 H -0.17922 0.13307 0.40350
H*4 H -0.30721 0.16127 0.14340
O5 O -0.42312 0.35226 0.22015
H*6 H -0.34071 0.43783 0.20993
N1 N 0.21994 0.35563 0.24514
H*2 H 0.25684 0.42675 0.14844
H*3 H 0.06808 0.40718 0.18217
H*4 H 0.24664 0.21612 0.25850
O5 O 0.34995 0.39025 0.43645
H*6 H 0.31973 0.32488 0.53319
N'1+ N -0.37837 0.00684 0.75428
N2+ N -0.22133 0.20792 0.89615
N'3+ N -0.35979 0.10564 0.87943
N'4+ N -0.25733 0.04107 0.68918
C5+ C -0.15764 0.16721 0.77706
C6+ C -0.00911 0.24325 0.74632
N'7+ N 0.04140 0.19150 0.62376
N'8+ N 0.17904 0.28910 0.63449
N'9+ N 0.21037 0.39494 0.75774
N'10+ N 0.09382 0.36929 0.83098
O11+ O -0.16934 0.32009 1.00897

#END

data_2NH3OH_BTO_1_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                 11.673
_cell_length_b                 17.104
_cell_length_c                 4.265
_cell_angle_alpha               90.00
_cell_angle_beta                92.62
_cell_angle_gamma                 90.00
_cell_volume                   850.638
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.02140 0.87268 0.54641
H*2 H -0.04133 0.81493 0.58637
H*3 H -0.07978 0.90769 0.65513
H*4 H 0.06094 0.88339 0.63503
O5 O -0.03013 0.88075 0.21816
H*6 H -0.01178 0.93502 0.16996
N1 N 0.05930 0.64233 -0.71167
H*2 H 0.00346 0.62301 -0.88921
H*3 H 0.01354 0.67306 -0.55062
H*4 H 0.09954 0.59456 -0.60734
O5 O 0.13719 0.69058 -0.86270
H*6 H 0.19199 0.71024 -0.70164
N'1+ N 0.17457 0.53728 -0.32082
N2+ N 0.30986 0.48493 -0.03148
N'3+ N 0.28401 0.54499 -0.23054
N'4+ N 0.12843 0.47454 -0.18805
C5+ C 0.21243 0.44103 -0.00551
C6+ C 0.19819 0.37036 0.18284
N'7+ N 0.09668 0.33194 0.18889
N'8+ N 0.11730 0.27148 0.38372
N'9+ N 0.22615 0.27322 0.49057
N'10+ N 0.27968 0.33498 0.36819
O11+ O 0.41142 0.47605 0.09839

#END

data_2NH3OH_BTO_1_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                 18.586
_cell_length_b                 12.055
_cell_length_c                 7.691
_cell_angle_alpha               90.00
_cell_angle_beta                90.00
_cell_angle_gamma                 90.00
_cell_volume                   1723.2
loop_
_atom_site_label
```

_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.86452 0.04124 -0.03500
H*2 H 0.81915 0.09035 -0.03118
H*3 H 0.85072 -0.03567 -0.08393
H*4 H 0.90255 0.07907 -0.11293
O5 O 0.88734 0.03464 0.13898
H*6 H 0.93052 -0.01150 0.14115
N1 N 0.10660 0.54576 0.00387
H*2 H 0.06949 0.50710 -0.07514
H*3 H 0.08019 0.60255 0.08159
H*4 H 0.13214 0.48646 0.07865
O5 O 0.15445 0.59784 -0.11181
H*6 H 0.19074 0.63571 -0.04173
N'1+ N 0.47182 0.17221 -0.32424
N2+ N 0.52997 0.32170 -0.26257
N'3+ N 0.46743 0.28178 -0.32903
N'4+ N 0.53477 0.13950 -0.25726
C5+ C 0.57191 0.23255 -0.21787
C6+ C 0.64406 0.23409 -0.14116
N'7+ N 0.68025 0.13954 -0.10258
N'8+ N 0.74303 0.17422 -0.03586
N'9+ N 0.74476 0.28456 -0.03414
N'10+ N 0.68304 0.32500 -0.09981
O11+ O 0.54238 0.42702 -0.24949

#END

S57. Optimized crystal structure coordinates for 5 polymorphs of **8c** (ionic form).

data_2N2H5_BTO_1_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 4.073
_cell_length_b 16.483
_cell_length_c 13.300
_cell_angle_alpha 90.00
_cell_angle_beta 104.34
_cell_angle_gamma 90.00
_cell_volume 865.079
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x

```
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.41536 -0.09916 0.53238
H*2 H 0.60958 -0.06143 0.56891
H*3 H 0.34610 -0.13185 0.58972
N4 N 0.54693 -0.15532 0.46829
H*5 H 0.35363 -0.19312 0.43322
H*6 H 0.61861 -0.12231 0.41229
H*7 H 0.21220 -0.06406 0.49450
N1 N 0.13267 0.85797 0.05129
H*2 H -0.04555 0.81773 0.01133
H*3 H 0.26966 0.87716 0.00033
N4 N 0.35958 0.81436 0.13484
H*5 H 0.53791 0.85451 0.17339
H*6 H 0.22089 0.79474 0.18445
H*7 H 0.00932 0.90729 0.07283
N'1+ N -0.13545 0.05591 0.84949
N2+ N -0.01520 0.00032 0.71643
N'3+ N -0.17972 0.06339 0.74789
N'4+ N 0.05139 -0.00956 0.88515
C5+ C 0.12890 -0.04514 0.80241
C6+ C 0.33165 -0.11911 0.80723
N'7+ N 0.46111 -0.15880 0.89769
N'8+ N 0.62783 -0.22226 0.87108
N'9+ N 0.60058 -0.22104 0.76931
N'10+ N 0.41497 -0.15663 0.72662
O11+ O -0.01092 -0.00955 0.62021

#END

data_2N2H5_BTO_1_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                 9.895
_cell_length_b                 12.659
_cell_length_c                 7.702
_cell_angle_alpha               90.00
_cell_angle_beta                63.51
_cell_angle_gamma                 90.00
_cell_volume                   863.471
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.27062 -0.08814 -0.05844
H*2 H 0.23185 -0.13185 -0.13962
H*3 H 0.17716 -0.05571 0.05383
N4 N 0.36232 -0.00278 -0.17842
H*5 H 0.39895 0.04091 -0.09613
H*6 H 0.45395 -0.03567 -0.29069
H*7 H 0.32296 -0.13829 -0.00145
N1 N 0.20178 0.49864 -0.02856
H*2 H 0.26865 0.44216 -0.00936
H*3 H 0.16608 0.46757 -0.12449
N4 N 0.29490 0.59000 -0.11848
H*5 H 0.22810 0.64522 -0.13902
H*6 H 0.33126 0.61966 -0.02324
H*7 H 0.10865 0.51171 0.10260
N'1+ N -0.08761 0.22642 0.67440
N2+ N 0.05251 0.35459 0.68293
N'3+ N -0.09011 0.32795 0.71701
N'4+ N 0.05109 0.18618 0.61401
C5+ C 0.14042 0.26581 0.61859
C6+ C 0.30197 0.25560 0.56335
N'7+ N 0.37664 0.16277 0.50152
N'8+ N 0.51945 0.18456 0.46539
N'9+ N 0.53070 0.28580 0.50353
N'10+ N 0.39529 0.33296 0.56574
O11+ O 0.08732 0.44950 0.71103

#END

data_2N2H5_BTO_1_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                 13.600
_cell_length_b                 14.146
_cell_length_c                 4.830
_cell_angle_alpha               90.00
_cell_angle_beta                74.92
_cell_angle_gamma                 90.00
_cell_volume                   897.223
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.37562 -0.38157 0.64189
H*2 H 0.42985 -0.40392 0.74120
H*3 H 0.40101 -0.40091 0.42994
N4 N 0.37124 -0.27934 0.65584
H*5 H 0.31807 -0.25768 0.55402
H*6 H 0.34707 -0.26070 0.86705
H*7 H 0.30830 -0.41669 0.73166
N1 N 0.43408 0.14550 -0.48558
H*2 H 0.44189 0.20371 -0.61717
H*3 H 0.43122 0.08749 -0.61166
N4 N 0.33738 0.15282 -0.27226
H*5 H 0.32971 0.09428 -0.14454
H*6 H 0.34043 0.21116 -0.15008
H*7 H 0.49782 0.14017 -0.40796
N'1+ N 0.09649 -0.18767 0.74290
N2+ N 0.13307 -0.04603 0.84624
N'3+ N 0.07024 -0.09802 0.72899
N'4+ N 0.17392 -0.19584 0.86462
C5+ C 0.19775 -0.10740 0.93075
C6+ C 0.27889 -0.08437 1.06826
N'7+ N 0.33812 -0.15195 1.14206
N'8+ N 0.40224 -0.10423 1.26004
N'9+ N 0.38275 -0.01210 1.25777
N'10+ N 0.30522 0.00287 1.13802
O11+ O 0.12660 0.04516 0.86459

#END

data_2N2H5_BTO_1_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                 3.906
_cell_length_b                 29.795
_cell_length_c                 7.285
_cell_angle_alpha               90.00
_cell_angle_beta                79.96
_cell_angle_gamma                 90.00
_cell_volume                   834.84
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

```
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.24761 0.43402 0.80378
H*2 H 0.07451 0.42894 0.92557
H*3 H 0.41637 0.40724 0.78944
N4 N 0.44440 0.47431 0.82510
H*5 H 0.61823 0.47884 0.70444
H*6 H 0.27442 0.50065 0.84134
H*7 H 0.11287 0.43384 0.69374
N1 N 0.13682 0.18543 -0.87219
H*2 H 0.27802 0.18212 -1.00455
H*3 H -0.04767 0.16043 -0.85637
N4 N -0.04124 0.22823 -0.86094
H*5 H -0.18383 0.23102 -0.72984
H*6 H 0.14372 0.25284 -0.87887
H*7 H 0.30049 0.18030 -0.77706
N'1+ N -0.02740 -0.03935 0.18875
N2+ N 0.23359 -0.09729 0.05348
N'3+ N 0.06673 -0.05867 0.02401
N'4+ N 0.07193 -0.06393 0.32392
C5+ C 0.23633 -0.10047 0.24104
C6+ C 0.38691 -0.13629 0.33946
N'7+ N 0.37267 -0.13558 0.52680
N'8+ N 0.53510 -0.17329 0.56418
N'9+ N 0.64260 -0.19577 0.40689
N'10+ N 0.55312 -0.17331 0.26224
O11+ O 0.35844 -0.12405 -0.08167

#END

data_2N2H5_BTO_1_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a                 13.359
_cell_length_b                 13.579
_cell_length_c                 4.964
_cell_angle_alpha               90.00
_cell_angle_beta                107.44
_cell_angle_gamma                90.00
_cell_volume                   859.085
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
```

_atom_site_fract_y
_atom_site_fract_z
N1 N 0.39289 -0.12032 0.85072
H*2 H 0.37778 -0.18532 0.73943
H*3 H 0.44624 -0.08237 0.77798
N4 N 0.44221 -0.14369 1.14541
H*5 H 0.45802 -0.07876 1.25390
H*6 H 0.38917 -0.18230 1.21513
H*7 H 0.32434 -0.07993 0.80589
N1 N 0.08069 0.83247 0.05995
H*2 H 0.07622 0.76696 -0.04708
H*3 H 0.08244 0.88749 -0.08101
N4 N 0.17921 0.83426 0.28464
H*5 H 0.18357 0.89997 0.38781
H*6 H 0.17732 0.77875 0.42194
H*7 H 0.01372 0.84048 0.12099
N'1+ N 0.11919 0.00066 0.79668
N2+ N 0.13297 0.13872 0.59696
N'3+ N 0.07683 0.08933 0.74088
N'4+ N 0.20062 -0.00939 0.69454
C5+ C 0.21026 0.07679 0.56840
C6+ C 0.29024 0.09727 0.42847
N'7+ N 0.36295 0.02939 0.41417
N'8+ N 0.42115 0.07455 0.27285
N'9+ N 0.38537 0.16548 0.20481
N'10+ N 0.30266 0.18220 0.30003
O11+ O 0.11081 0.22838 0.51127

#END

S58. Optimized crystal structure coordinates for 5 polymorphs of **8d** (ionic form).

data_2GH_BTO_1_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 3.584
_cell_length_b 31.862
_cell_length_c 9.501
_cell_angle_alpha 90.00
_cell_angle_beta 82.85
_cell_angle_gamma 90.00
_cell_volume 1076.51
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x

```
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.51741 0.54300 0.48876
N2 N 0.66439 0.58130 0.46485
H*3 H 0.81367 0.58878 0.37088
H*4 H 0.63046 0.60388 0.54006
N5 N 0.56677 0.51373 0.38727
H*6 H 0.45814 0.48459 0.40311
H*7 H 0.71414 0.51988 0.29178
N8 N 0.32107 0.53397 0.61416
H*9 H 0.28042 0.55562 0.69229
H*10 H 0.20763 0.50524 0.63444
C1 C 0.57447 0.20589 0.35211
N2 N 0.69072 0.16601 0.35231
H*3 H 0.71210 0.14834 0.26333
H*4 H 0.76059 0.15238 0.44144
N5 N 0.48383 0.22313 0.23258
H*6 H 0.39536 0.25320 0.23009
H*7 H 0.50115 0.20658 0.14126
N8 N 0.54886 0.22854 0.47144
H*9 H 0.61595 0.21613 0.56291
H*10 H 0.46167 0.25872 0.47363
N'1+ N -0.14617 0.15157 0.63924
N2+ N -0.30101 0.17464 0.85162
N'3+ N -0.21271 0.18641 0.71415
N'4+ N -0.18790 0.11767 0.72279
C5+ C -0.28522 0.13166 0.85661
C6+ C -0.35829 0.10462 0.98172
N'7+ N -0.33325 0.06221 0.97276
N'8+ N -0.41841 0.04876 1.10671
N'9+ N -0.49155 0.08149 1.19270
N'10+ N -0.45607 0.11727 1.11710
O11+ O -0.38158 0.20178 0.95219

#END

data_2GH_BTO_1_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P c'
_symmetry_Int_Tables_number      7
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 x,-y,1/2+z
_cell_length_a                 3.632
_cell_length_b                 15.907
_cell_length_c                 9.145
_cell_angle_alpha               90.00
_cell_angle_beta                95.11
_cell_angle_gamma                90.00
_cell_volume                   526.245
```

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.02863 0.41438 0.32272
N2 N 0.09689 0.45927 0.44039
H*3 H 0.25439 0.43269 0.52465
H*4 H 0.03791 0.52109 0.44849
N5 N 0.05377 0.33265 0.31495
H*6 H -0.03822 0.29758 0.22705
H*7 H 0.21042 0.30359 0.39674
N8 N -0.23655 0.45121 0.21282
H*9 H -0.30207 0.51288 0.21646
H*10 H -0.33422 0.41846 0.12292
C1 C -0.98369 0.91651 -0.00501
N2 N -0.78434 0.93424 0.12127
H*3 H -0.67949 0.99233 0.14180
H*4 H -0.73272 0.89007 0.19985
N5 N -1.04768 0.97621 -0.10707
H*6 H -1.19758 0.96416 -0.20323
H*7 H -0.94799 1.03512 -0.09101
N8 N -1.11906 0.83908 -0.02923
H*9 H -1.07400 0.79304 0.04640
H*10 H -1.27036 0.82434 -0.12387
N'1+ N -0.64051 0.30550 -0.38589
N2+ N -0.44066 0.34706 -0.16904
N'3+ N -0.50794 0.37176 -0.31102
N'4+ N -0.66184 0.23878 -0.29797
C5+ C -0.53717 0.26392 -0.16131
C6+ C -0.51393 0.20987 -0.03111
N'7+ N -0.61873 0.12803 -0.03775
N'8+ N -0.55778 0.10014 0.10072
N'9+ N -0.42247 0.16217 0.18711
N'10+ N -0.39132 0.23239 0.10725
O11+ O -0.30831 0.39809 -0.06733

#END

data_2GH_BTO_1_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                  32.115
```

```
_cell_length_b                  3.660
_cell_length_c                  8.940
_cell_angle_alpha                 90.00
_cell_angle_beta                90.00
_cell_angle_gamma                   90.00
_cell_volume                    1050.82
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.28996 -0.09737 0.06445
N2 N 0.25950 -0.16718 -0.03347
H*3 H 0.23035 -0.07069 -0.01765
H*4 H 0.26475 -0.31846 -0.12613
N5 N 0.28213 0.10368 0.18615
H*6 H 0.30469 0.15967 0.26155
H*7 H 0.25342 0.20548 0.20627
N8 N 0.32825 -0.22861 0.04067
H*9 H 0.33485 -0.38110 -0.05055
H*10 H 0.35172 -0.17913 0.11321
C1 C 0.54377 0.17762 0.39129
N2 N 0.58420 0.09209 0.38397
H*3 H 0.60170 0.16213 0.29451
H*4 H 0.59844 -0.04509 0.46769
N5 N 0.52574 0.35934 0.27882
H*6 H 0.49524 0.42668 0.28208
H*7 H 0.54210 0.43462 0.18730
N8 N 0.52136 0.08143 0.51108
H*9 H 0.53437 -0.05595 0.59729
H*10 H 0.49078 0.14333 0.51888
N'1+ N 0.10032 0.15836 -0.31401
N2+ N 0.07745 0.35537 -0.10234
N'3+ N 0.06624 0.27126 -0.24468
N'4+ N 0.13320 0.16598 -0.22217
C5+ C 0.11932 0.28924 -0.08869
C6+ C 0.14543 0.33922 0.04411
N'7+ N 0.18677 0.26353 0.04344
N'8+ N 0.19962 0.34228 0.18253
N'9+ N 0.16757 0.46008 0.26358
N'10+ N 0.13286 0.46147 0.17945
O11+ O 0.05082 0.47504 -0.00534

#END

data_2GH_BTO_1_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                32.466
_cell_length_b                3.601
_cell_length_c                9.257
_cell_angle_alpha              90.00
_cell_angle_beta               90.00
_cell_angle_gamma               90.00
_cell_volume                  1082.24
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.79511 0.17003 0.63172
N2 N 0.78487 0.33058 0.75695
H*3 H 0.75559 0.40993 0.77751
H*4 H 0.80611 0.37724 0.83467
N5 N 0.76636 0.11167 0.53078
H*6 H 0.77343 -0.00919 0.43542
H*7 H 0.73672 0.18673 0.54691
N8 N 0.83410 0.06784 0.60743
H*9 H 0.85630 0.10935 0.68223
H*10 H 0.84250 -0.05389 0.51358
C1 C 0.54272 0.31549 -0.00962
N2 N 0.58178 0.43189 -0.00246
H*3 H 0.59999 0.43621 -0.09099
H*4 H 0.59424 0.51894 0.09170
N5 N 0.52705 0.20182 -0.13570
H*6 H 0.49761 0.11279 -0.14351
H*7 H 0.54418 0.20162 -0.22684
N8 N 0.51933 0.31276 0.10930
H*9 H 0.53056 0.39747 0.20564
H*10 H 0.48974 0.22591 0.10629
N'1+ N 0.10048 -0.12747 0.71423
N2+ N 0.07693 0.02615 0.50503
N'3+ N 0.06595 -0.06936 0.64160
N'4+ N 0.13344 -0.07336 0.63006
C5+ C 0.11913 0.02336 0.49823
C6+ C 0.14517 0.10787 0.37323
N'7+ N 0.18688 0.09529 0.38026
N'8+ N 0.19952 0.18807 0.24710
N'9+ N 0.16701 0.25371 0.16341
N'10+ N 0.13218 0.20550 0.23979
O11+ O 0.04985 0.10129 0.40667

#END
```

```
data_2GH_BTO_1_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                 3.583
_cell_length_b                 28.747
_cell_length_c                 10.632
_cell_angle_alpha               90.00
_cell_angle_beta                78.95
_cell_angle_gamma                 90.00
_cell_volume                   1074.8
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.17639 -0.21752 0.53820
N2 N -0.05506 -0.17343 0.53125
H*3 H 0.00896 -0.15703 0.60848
H*4 H -0.02384 -0.15523 0.44858
N5 N -0.21506 -0.24077 0.64889
H*6 H -0.30629 -0.27410 0.65624
H*7 H -0.15418 -0.22569 0.72842
N8 N -0.25906 -0.23836 0.43445
H*9 H -0.23184 -0.22143 0.34988
H*10 H -0.35115 -0.27164 0.43760
C1 C -0.16477 0.53503 -0.03286
N2 N -0.05883 0.57790 -0.00569
H*3 H 0.08974 0.59862 -0.07429
H*4 H -0.12425 0.59083 0.08423
N5 N -0.07425 0.51882 -0.15274
H*6 H -0.15148 0.48653 -0.17535
H*7 H 0.07402 0.53838 -0.22422
N8 N -0.36123 0.50837 0.05985
H*9 H -0.43258 0.51994 0.15106
H*10 H -0.44408 0.47588 0.04141
N'1+ N 0.04795 0.06721 0.28198
N2+ N 0.02603 0.13926 0.33865
N'3+ N 0.06860 0.11017 0.23627
N'4+ N -0.00635 0.06731 0.41003
C5+ C -0.02074 0.11235 0.44706
C6+ C -0.07684 0.12808 0.58042
N'7+ N -0.11996 0.09781 0.68000
N'8+ N -0.16354 0.12485 0.78463
```

N'9+ N -0.14756 0.16940 0.75002
N'10+ N -0.09300 0.17266 0.62161
O11+ O 0.03288 0.18403 0.32557

#END

S59. Optimized crystal structure coordinates for 5 polymorphs of **8e** (ionic form).

data_2AGH_BTO_1_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 8.938
_cell_length_b 11.127
_cell_length_c 12.838
_cell_angle_alpha 90.00
_cell_angle_beta 101.80
_cell_angle_gamma 90.00
_cell_volume 1249.8
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.70844 0.36647 -0.41004
N2 N 0.76572 0.44663 -0.46927
H*3 H 0.83214 0.42078 -0.52017
H*4 H 0.74400 0.53533 -0.46462
N5 N 0.74011 0.24902 -0.41859
H*6 H 0.80675 0.22246 -0.46957
N7 N 0.62106 0.40059 -0.34307
H*8 H 0.59481 0.48780 -0.33446
H*9 H 0.58065 0.33624 -0.30012
N10 N 0.67995 0.16571 -0.35651
H*11 H 0.61064 0.10636 -0.40402
H*12 H 0.76601 0.12121 -0.30728
C1 C 0.11150 0.55531 0.11470
N2 N 0.20110 0.47416 0.08038
H*3 H 0.25733 0.49381 0.02178
H*4 H 0.21490 0.39091 0.11225
N5 N 0.09615 0.66533 0.07012
H*6 H 0.15231 0.68564 0.01123
N7 N 0.03756 0.52937 0.19182
H*8 H 0.04623 0.44789 0.22717
H*9 H -0.02877 0.59408 0.21479
N10 N 0.00240 0.74972 0.10630

H*11 H 0.06469 0.82302 0.13652
H*12 H -0.08476 0.77455 0.04590
N'1+ N -0.21288 -0.16827 0.92051
N2+ N -0.11637 -0.05279 0.81673
N'3+ N -0.19048 -0.05407 0.89910
N'4+ N -0.15619 -0.24110 0.85522
C5+ C -0.09514 -0.16982 0.78953
C6+ C -0.02058 -0.21360 0.70527
N'7+ N -0.00660 -0.33250 0.68606
N'8+ N 0.06647 -0.33669 0.60468
N'9+ N 0.09536 -0.22558 0.57597
N'10+ N 0.04183 -0.14565 0.63794
O11+ O -0.07774 0.04653 0.77682

#END

data_2AGH_BTO_1_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 13.194
_cell_length_b 14.858
_cell_length_c 8.067
_cell_angle_alpha 90.00
_cell_angle_beta 53.15
_cell_angle_gamma 90.00
_cell_volume 1265.47
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.70666 0.34440 -0.23180
N2 N 0.66015 0.28082 -0.28700
H*3 H 0.70012 0.21915 -0.33333
H*4 H 0.58365 0.29284 -0.28380
N5 N 0.80882 0.32565 -0.23825
H*6 H 0.84941 0.26385 -0.28463
N7 N 0.65399 0.42552 -0.17086
H*8 H 0.57733 0.44209 -0.16400
H*9 H 0.69297 0.47116 -0.13075
N10 N 0.85697 0.39234 -0.18040
H*11 H 0.85316 0.37143 -0.05651
H*12 H 0.94780 0.40758 -0.30148

C1 C 0.45926 -0.24838 0.74834
N2 N 0.56086 -0.25992 0.74590
H*3 H 0.60921 -0.20688 0.74472
H*4 H 0.59196 -0.32214 0.74517
N5 N 0.42086 -0.16430 0.74923
H*6 H 0.46901 -0.11074 0.74806
N7 N 0.39571 -0.31823 0.74989
H*8 H 0.42161 -0.38224 0.74929
H*9 H 0.31948 -0.30572 0.75172
N10 N 0.31468 -0.15267 0.75178
H*11 H 0.24561 -0.11876 0.88176
H*12 H 0.33903 -0.11878 0.62287
N'1+ N 0.11062 0.45125 0.60503
N2+ N 0.17873 0.54452 0.72219
N'3+ N 0.10080 0.53564 0.66575
N'4+ N 0.19190 0.40505 0.61990
C5+ C 0.23550 0.46279 0.69333
C6+ C 0.32713 0.43937 0.73283
N'7+ N 0.37679 0.35552 0.69779
N'8+ N 0.45523 0.36036 0.75135
N'9+ N 0.45316 0.44324 0.81578
N'10+ N 0.37315 0.49487 0.80603
O11+ O 0.19042 0.61998 0.78946

#END

data_2AGH_BTO_1_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 8.641
_cell_length_b 9.448
_cell_length_c 12.894
_cell_angle_alpha 114.55
_cell_angle_beta 42.40
_cell_angle_gamma 112.86
_cell_volume 639.9
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.59250 0.28045 -0.13737
N2 N 0.52520 0.15229 -0.08592
H*3 H 0.42722 0.05748 -0.09681
H*4 H 0.57074 0.14698 -0.03470

N5 N 0.52810 0.28281 -0.20500
H*6 H 0.42968 0.18796 -0.21630
N7 N 0.72144 0.40516 -0.12298
H*8 H 0.77311 0.40779 -0.07295
H*9 H 0.76760 0.49909 -0.16392
N10 N 0.59892 0.41701 -0.25852
H*11 H 0.69828 0.38995 -0.37662
H*12 H 0.45851 0.46422 -0.20098
C1 C 0.20366 0.22083 0.56856
N2 N 0.19624 0.28014 0.68614
H*3 H 0.19189 0.39592 0.73542
H*4 H 0.19481 0.21052 0.72882
N5 N 0.20533 0.31765 0.51503
H*6 H 0.20098 0.43406 0.56402
N7 N 0.20939 0.06845 0.50378
H*8 H 0.20837 -0.00778 0.54072
H*9 H 0.21490 0.02970 0.41512
N10 N 0.21309 0.25501 0.39218
H*11 H 0.06965 0.27374 0.42803
H*12 H 0.35890 0.30398 0.29743
N'1+ N 0.11623 -0.30328 0.59101
N2+ N 0.21110 -0.10850 0.70681
N'3+ N 0.15831 -0.14813 0.62092
N'4+ N 0.13968 -0.36581 0.65417
C5+ C 0.19928 -0.24483 0.72736
C6+ C 0.24205 -0.26165 0.81221
N'7+ N 0.22467 -0.40404 0.82430
N'8+ N 0.27547 -0.37183 0.90880
N'9+ N 0.32144 -0.21723 0.94611
N'10+ N 0.30186 -0.14414 0.88687
O11+ O 0.26127 0.03625 0.75501

#END

data_2AGH_BTO_1_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 10.043
_cell_length_b 18.838
_cell_length_c 6.732
_cell_angle_alpha 90.00
_cell_angle_beta 108.99
_cell_angle_gamma 90.00
_cell_volume 1204.31

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.45222 0.42266 -0.04939
N2 N 0.34640 0.44952 -0.20882
H*3 H 0.35295 0.45326 -0.35507
H*4 H 0.25695 0.46681 -0.18706
N5 N 0.56972 0.40018 -0.08498
H*6 H 0.57697 0.40379 -0.23151
N7 N 0.44349 0.41776 0.14302
H*8 H 0.35714 0.43405 0.17581
H*9 H 0.52663 0.39701 0.25802
N10 N 0.67991 0.37217 0.08218
H*11 H 0.69882 0.32088 0.05166
H*12 H 0.76855 0.40195 0.10747
C1 C -0.13811 0.76751 0.15916
N2 N -0.01924 0.79928 0.27680
H*3 H -0.01208 0.85268 0.28988
H*4 H 0.06667 0.77062 0.35583
N5 N -0.25032 0.80764 0.05627
H*6 H -0.24381 0.86131 0.06875
N7 N -0.14743 0.69723 0.14205
H*8 H -0.06559 0.66538 0.21681
H*9 H -0.23987 0.67591 0.05096
N10 N -0.37419 0.77415 -0.06637
H*11 H -0.45478 0.78593 -0.01124
H*12 H -0.39885 0.78942 -0.21926
N'1+ N -0.08833 0.00730 0.70132
N2+ N 0.13773 0.01671 0.80709
N'3+ N 0.01549 0.05387 0.73591
N'4+ N -0.03818 -0.05861 0.74731
C5+ C 0.10378 -0.05356 0.81401
C6+ C 0.20028 -0.11383 0.88046
N'7+ N 0.15336 -0.18135 0.88022
N'8+ N 0.27068 -0.22075 0.94978
N'9+ N 0.38332 -0.17906 0.99023
N'10+ N 0.34254 -0.11116 0.94810
O11+ O 0.25942 0.04744 0.85553

#END

data_2AGH_BTO_1_5
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
```

2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 13.129
_cell_length_b 14.808
_cell_length_c 7.734
_cell_angle_alpha 90.00
_cell_angle_beta 121.93
_cell_angle_gamma 90.00
_cell_volume 1276.1
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.02269 0.74983 0.29418
N2 N -0.04298 0.66815 0.34452
H*3 H 0.00696 0.61401 0.35547
H*4 H -0.10893 0.65845 0.37296
N5 N 0.06612 0.75991 0.25745
H*6 H 0.11660 0.70581 0.26819
N7 N -0.08845 0.82103 0.27981
H*8 H -0.15580 0.81613 0.30621
H*9 H -0.06932 0.88131 0.24119
N10 N 0.08688 0.84539 0.20493
H*11 H 0.17141 0.86670 0.30996
H*12 H 0.07512 0.84368 0.06382
C1 C 0.29303 -0.35156 0.78180
N2 N 0.33933 -0.28701 0.72194
H*3 H 0.30243 -0.22476 0.68289
H*4 H 0.41259 -0.29887 0.71422
N5 N 0.19528 -0.33301 0.79003
H*6 H 0.15779 -0.27062 0.75101
N7 N 0.34166 -0.43346 0.83316
H*8 H 0.41495 -0.44990 0.82893
H*9 H 0.30305 -0.47981 0.87738
N10 N 0.14733 -0.40071 0.85267
H*11 H 0.14965 -0.38112 0.98095
H*12 H 0.06149 -0.41493 0.73942
N'1+ N 0.10779 0.44070 0.41333
N2+ N 0.18781 0.53861 0.31447
N'3+ N 0.10707 0.52751 0.37174
N'4+ N 0.18586 0.39507 0.38526
C5+ C 0.23687 0.45571 0.32310
C6+ C 0.32806 0.43382 0.27510
N'7+ N 0.36960 0.34856 0.28971
N'8+ N 0.45042 0.35550 0.23440
N'9+ N 0.45747 0.44094 0.18848
N'10+ N 0.38130 0.49221 0.21259
O11+ O 0.20813 0.61673 0.26356

#END
S60. Optimized crystal structure coordinates for 5 polymorphs of **8f** (ionic form).
data_2DAGH_BTO_1_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 16.176
_cell_length_b 12.031
_cell_length_c 7.533
_cell_angle_alpha 90.00
_cell_angle_beta 102.52
_cell_angle_gamma 90.00
_cell_volume 1431.16
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.53592 -0.10615 0.40334
N2 N 0.59271 -0.05223 0.32976
H*3 H 0.57747 -0.03747 0.19370
N4 N 0.46201 -0.13813 0.29549
H*5 H 0.41860 -0.17902 0.35000
N6 N 0.55246 -0.12781 0.58100
H*7 H 0.60887 -0.10220 0.65688
H*8 H 0.51080 -0.16830 0.63997
N9 N 0.44674 -0.11400 0.10938
N10 N 0.66945 -0.01919 0.44258
H*11 H 0.67529 0.06500 0.43853
H*12 H 0.43839 -0.18550 0.03536
H*13 H 0.39485 -0.06434 0.07308
H*14 H 0.71872 -0.05587 0.40090
C1 C 0.36350 0.35053 0.67287
N2 N 0.43071 0.38954 0.79278
H*3 H 0.47854 0.42360 0.74295
N4 N 0.36209 0.35795 0.49372
H*5 H 0.31145 0.32862 0.40186
N6 N 0.29890 0.30498 0.73034
H*7 H 0.30269 0.30116 0.86632
H*8 H 0.24749 0.27494 0.64293
N9 N 0.43106 0.40631 0.43816
N10 N 0.43181 0.38159 0.97887
H*11 H 0.43588 0.45891 1.03513
H*12 H 0.45841 0.35034 0.36729

H*13 H 0.41206 0.47474 0.36051
H*14 H 0.48212 0.33480 1.04190
N'1+ N 0.68561 -0.04456 0.01792
N2+ N 0.81994 -0.07568 0.07961
N'3+ N 0.75604 -0.02677 0.14173
N'4+ N 0.70136 -0.10310 -0.12208
C5+ C 0.78554 -0.12329 -0.08527
C6+ C 0.82959 -0.18540 -0.20423
N'7+ N 0.78816 -0.22873 -0.36522
N'8+ N 0.84872 -0.27851 -0.43331
N'9+ N 0.92330 -0.26592 -0.31893
N'10+ N 0.91345 -0.20746 -0.17277
O11+ O 0.89756 -0.07295 0.17082

#END

data_2DAGH_BTO_1_2
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P c'
_symmetry_Int_Tables_number 7
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 x,-y,1/2+z
_cell_length_a 8.149
_cell_length_b 7.433
_cell_length_c 19.773
_cell_angle_alpha 90.00
_cell_angle_beta 142.55
_cell_angle_gamma 90.00
_cell_volume 728.272
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.14208 0.05328 0.66478
N2 N 0.14515 0.11802 0.72896
H*3 H 0.31479 0.18262 0.80017
N4 N 0.36088 0.07613 0.69679
H*5 H 0.36043 0.02756 0.64871
N6 N -0.07484 -0.03260 0.57049
H*7 H -0.23477 -0.04666 0.54971
H*8 H -0.08253 -0.08272 0.52057
N9 N 0.58531 0.16704 0.79638
N10 N -0.08293 0.09385 0.69525
H*11 H -0.15829 0.21569 0.68469
H*12 H 0.74968 0.08486 0.85030
H*13 H 0.62378 0.27965 0.78128
H*14 H -0.03269 0.02135 0.75354

C1 C -0.31268 0.55525 -0.04324
N2 N -0.33810 0.63286 -0.11232
H*3 H -0.51289 0.69937 -0.17949
N4 N -0.51693 0.56834 -0.06532
H*5 H -0.49951 0.50998 -0.01346
N6 N -0.08802 0.46626 0.04616
H*7 H 0.06036 0.45987 0.05948
H*8 H -0.06356 0.40652 0.09959
N9 N -0.75008 0.66287 -0.16000
N10 N -0.12506 0.61879 -0.08893
H*11 H -0.05551 0.74368 -0.07822
H*12 H -0.91346 0.57986 -0.21244
H*13 H -0.77929 0.76913 -0.13791
H*14 H -0.18936 0.55485 -0.15257
N'1+ N 0.07567 -0.04714 -0.06384
N2+ N 0.33053 0.12434 -0.04074
N'3+ N 0.17127 -0.02425 -0.09449
N'4+ N 0.16675 0.08084 0.00771
C5+ C 0.32722 0.18964 0.02304
C6+ C 0.46866 0.34786 0.09570
N'7+ N 0.44905 0.39898 0.15495
N'8+ N 0.60381 0.54654 0.21019
N'9+ N 0.71200 0.58304 0.18556
N'10+ N 0.63068 0.46007 0.11341
O11+ O 0.45468 0.18270 -0.05337

#END

data_2DAGH_BTO_1_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 13.282
_cell_length_b 15.334
_cell_length_c 7.218
_cell_angle_alpha 118.23
_cell_angle_beta 89.18
_cell_angle_gamma 138.94
_cell_volume 685.928
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.25289 -0.00313 -0.20914
N2 N -0.31003 -0.06711 -0.09766

H*3 H -0.36116 -0.05111 -0.00736
N4 N -0.26536 0.07863 -0.19713
H*5 H -0.22242 0.12752 -0.28101
N6 N -0.18462 -0.02027 -0.33029
H*7 H -0.17784 -0.08271 -0.33450
H*8 H -0.14057 0.02671 -0.41593
N9 N -0.33782 0.09429 -0.06824
N10 N -0.29672 -0.15199 -0.11079
H*11 H -0.42823 -0.28635 -0.20570
H*12 H -0.23818 0.23117 0.08474
H*13 H -0.45719 0.02386 -0.19412
H*14 H -0.20973 -0.07953 0.07251
C1 C 0.33204 0.58250 0.25983
N2 N 0.38385 0.53560 0.15294
H*3 H 0.44344 0.57984 0.06792
N4 N 0.36063 0.68492 0.25036
H*5 H 0.32184 0.72112 0.33080
N6 N 0.25322 0.52839 0.37399
H*7 H 0.23443 0.45155 0.37653
H*8 H 0.21285 0.56179 0.45605
N9 N 0.44381 0.73935 0.12885
N10 N 0.35377 0.42910 0.16339
H*11 H 0.48020 0.50140 0.26248
H*12 H 0.35316 0.68546 -0.02512
H*13 H 0.56834 0.88126 0.25872
H*14 H 0.26552 0.30605 -0.02070
N'1+ N -0.27756 0.18633 0.49498
N2+ N 0.01218 0.41786 0.62523
N'3+ N -0.13627 0.35695 0.59259
N'4+ N -0.22651 0.13422 0.46305
C5+ C -0.04473 0.27831 0.54408
C6+ C 0.06645 0.27932 0.54217
N'7+ N -0.00646 0.13149 0.45648
N'8+ N 0.13530 0.18425 0.48446
N'9+ N 0.28687 0.35593 0.58246
N'10+ N 0.24814 0.42006 0.62122
O11+ O 0.17315 0.58154 0.71830

#END

data_2DAGH_BTO_1_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 17.713

```
_cell_length_b                    11.739
_cell_length_c                    7.420
_cell_angle_alpha                 90.00
_cell_angle_beta                  104.69
_cell_angle_gamma                 90.00
_cell_volume                      1492.43
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.48071 0.60018 0.62775
N2 N 0.43689 0.54244 0.71944
H*3 H 0.46412 0.50827 0.84499
N4 N 0.55796 0.61042 0.70462
H*5 H 0.59163 0.65401 0.63620
N6 N 0.44817 0.64683 0.46259
H*7 H 0.38986 0.63697 0.41012
H*8 H 0.47983 0.69078 0.39052
N9 N 0.59019 0.56031 0.87838
N10 N 0.35660 0.53208 0.63881
H*11 H 0.32613 0.56799 0.72363
H*12 H 0.63073 0.50093 0.86770
H*13 H 0.61484 0.62088 0.97333
H*14 H 0.34198 0.44832 0.61825
C1 C 0.56531 0.12087 0.27125
N2 N 0.63628 0.11731 0.38947
H*3 H 0.68327 0.12024 0.33438
N4 N 0.55921 0.12808 0.08681
H*5 H 0.50569 0.13082 -0.00382
N6 N 0.50160 0.11731 0.33555
H*7 H 0.50898 0.11189 0.47533
H*8 H 0.44742 0.11986 0.24955
N9 N 0.62738 0.13164 0.02414
N10 N 0.64225 0.10982 0.58109
H*11 H 0.67152 0.17874 0.64757
H*12 H 0.62938 0.06375 -0.05989
H*13 H 0.62992 0.20570 -0.04548
H*14 H 0.67098 0.03712 0.63320
N'1+ N 0.29463 0.06864 1.17966
N2+ N 0.23353 0.15596 0.92984
N'3+ N 0.22435 0.10174 1.08453
N'4+ N 0.34902 0.09930 1.09268
C5+ C 0.31151 0.15427 0.93541
C6+ C 0.34967 0.20222 0.79893
N'7+ N 0.42787 0.19497 0.82036
N'8+ N 0.44042 0.24764 0.67016
N'9+ N 0.37300 0.28500 0.56285
N'10+ N 0.31448 0.25770 0.64022
O11+ O 0.17500 0.19871 0.80727
```

```
#END

data_2DAGH_BTO_1_5
_symmetry_cell_setting          triclinic
_symmetry_space_group_name_H-M   'P -1'
_symmetry_Int_Tables_number      2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 11.684
_cell_length_b                 12.459
_cell_length_c                 7.440
_cell_angle_alpha               137.87
_cell_angle_beta                89.01
_cell_angle_gamma                80.82
_cell_volume                   702.024
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.39443 0.36961 0.25599
N2 N 0.43243 0.24315 0.21189
H*3 H 0.46106 0.12771 0.01453
N4 N 0.39570 0.33903 0.04000
H*5 H 0.36708 0.43404 0.07138
N6 N 0.35589 0.52365 0.51045
H*7 H 0.35652 0.54083 0.66665
H*8 H 0.32677 0.62121 0.54949
N9 N 0.43678 0.17565 -0.22458
N10 N 0.43091 0.27571 0.43728
H*11 H 0.51460 0.23875 0.43958
H*12 H 0.37148 0.14029 -0.33413
H*13 H 0.50870 0.16457 -0.32117
H*14 H 0.37770 0.21453 0.42664
C1 C 0.00002 0.46110 1.20075
N2 N 0.08302 0.54569 1.30293
H*3 H 0.16516 0.48666 1.27253
N4 N 0.02841 0.30351 1.06384
H*5 H -0.03388 0.23844 0.98570
N6 N -0.10922 0.53216 1.23432
H*7 H -0.12658 0.65092 1.33866
H*8 H -0.17346 0.47125 1.15944
N9 N 0.14406 0.23276 1.03243
N10 N 0.05297 0.70950 1.44508
H*11 H 0.10423 0.72014 1.34910
H*12 H 0.14353 0.19941 1.12259
H*13 H 0.18277 0.13245 0.83028
H*14 H 0.06508 0.78695 1.64073
```

N'1+ N 0.13651 0.92554 -0.04985
N2+ N 0.22576 1.04189 0.28640
N'3+ N 0.17109 1.06186 0.15013
N'4+ N 0.16664 0.81793 -0.04858
C5+ C 0.22281 0.88932 0.16165
C6+ C 0.27067 0.81284 0.23588
N'7+ N 0.26210 0.66005 0.09538
N'8+ N 0.31515 0.63353 0.22213
N'9+ N 0.35399 0.76411 0.42958
N'10+ N 0.32732 0.87967 0.44396
O11+ O 0.26990 1.15487 0.49508

#END

S61. Optimized crystal structure coordinates for 5 polymorphs of **8g** (ionic form).

data_2TAGH_BTO_1_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 12.131
_cell_length_b 10.469
_cell_length_c 7.702
_cell_angle_alpha 89.23
_cell_angle_beta 93.04
_cell_angle_gamma 125.06
_cell_volume 799.365
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.29868 0.12385 -0.01684
N2 N 0.43380 0.21843 -0.00893
H*3 H 0.47783 0.33517 -0.01621
N4 N 0.23552 -0.03107 -0.00784
H*5 H 0.29369 -0.07219 0.00495
N6 N 0.22672 0.18419 -0.03375
H*7 H 0.12452 0.10857 -0.03926
N8 N 0.09421 -0.12741 -0.01640
N9 N 0.50669 0.15247 0.00875
H*10 H 0.56620 0.19253 0.12076
H*11 H 0.05949 -0.20178 -0.12104
H*12 H 0.06064 -0.18976 0.09443
H*13 H 0.56505 0.18052 -0.09471
N14 N 0.29514 0.34650 -0.04287
H*15 H 0.26977 0.37478 -0.15798
H*16 H 0.27092 0.38680 0.05749

```
C1 C 0.30581 0.14588 0.48112
N2 N 0.43185 0.18411 0.50267
H*3 H 0.44377 0.09561 0.50801
N4 N 0.28447 0.25812 0.47321
H*5 H 0.36649 0.37074 0.48409
N6 N 0.20112 -0.00459 0.46748
H*7 H 0.10717 -0.02871 0.45126
N8 N 0.15178 0.21510 0.45062
N9 N 0.53954 0.34222 0.51659
H*10 H 0.60259 0.37007 0.41873
H*11 H 0.12938 0.25497 0.55344
H*12 H 0.14066 0.26041 0.33865
H*13 H 0.59132 0.36463 0.63352
N14 N 0.22611 -0.11969 0.47615
H*15 H 0.17982 -0.19012 0.57858
H*16 H 0.19109 -0.18468 0.36379
N'1+ N -0.28339 0.32916 0.26787
N2+ N -0.10764 0.56689 0.27102
N'3+ N -0.24358 0.47590 0.28268
N'4+ N -0.17855 0.32144 0.24705
C5+ C -0.06736 0.46996 0.24875
C6+ C 0.06992 0.51429 0.22975
N'7+ N 0.09692 0.40664 0.20835
N'8+ N 0.23102 0.49064 0.19597
N'9+ N 0.28276 0.64200 0.20925
N'10+ N 0.18366 0.66099 0.23071
O11+ O -0.03788 0.71768 0.28083

#END

data_2TAGH_BTO_1_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                 12.107
_cell_length_b                 7.707
_cell_length_c                 10.463
_cell_angle_alpha               90.85
_cell_angle_beta                55.02
_cell_angle_gamma                93.44
_cell_volume                   798.254
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

C1 C 0.69304 0.51845 0.14645
N2 N 0.56662 0.49466 0.18525
H*3 H 0.55412 0.48918 0.09710
N4 N 0.71514 0.52664 0.25820
H*5 H 0.63337 0.51424 0.37091
N6 N 0.79736 0.53405 -0.00410
H*7 H 0.89163 0.55193 -0.02866
N8 N 0.84822 0.55159 0.21460
N9 N 0.45932 0.47874 0.34344
H*10 H 0.40798 0.36099 0.36550
H*11 H 0.85910 0.66360 0.26026
H*12 H 0.87152 0.44924 0.25365
H*13 H 0.39556 0.57536 0.37210
N14 N 0.77158 0.52503 -0.11869
H*15 H 0.80583 0.63794 -0.18310
H*16 H 0.81825 0.42357 -0.18971
C1 C 0.70134 0.01509 0.12337
N2 N 0.77363 0.03510 0.18348
H*3 H 0.87596 0.04206 0.10781
N4 N 0.56603 0.00517 0.21803
H*5 H 0.52211 0.01336 0.33464
N6 N 0.76436 0.00500 -0.03140
H*7 H 0.70594 -0.01015 -0.07234
N8 N 0.49280 -0.01574 0.15231
N9 N 0.70535 0.04529 0.34563
H*10 H 0.73046 0.16150 0.37312
H*11 H 0.43359 -0.12854 0.19312
H*12 H 0.43394 0.08649 0.17972
H*13 H 0.73011 -0.05353 0.38652
N14 N 0.90587 0.01572 -0.12783
H*15 H 0.93980 -0.09520 -0.18943
H*16 H 0.94015 0.11983 -0.20283
N'1+ N -0.28170 0.27473 0.66846
N2+ N -0.10641 0.27369 0.43071
N'3+ N -0.24205 0.28873 0.52172
N'4+ N -0.17705 0.25118 0.67615
C5+ C -0.06615 0.25024 0.52762
C6+ C 0.07086 0.22776 0.48326
N'7+ N 0.09788 0.20549 0.59089
N'8+ N 0.23169 0.18977 0.50687
N'9+ N 0.28324 0.20194 0.35552
N'10+ N 0.18431 0.22599 0.33655
O11+ O -0.03687 0.28193 0.27993

#END

data_2TAGH_BTO_1_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                 21.332
_cell_length_b                 10.493
_cell_length_c                 7.830
_cell_angle_alpha               90.00
_cell_angle_beta                111.52
_cell_angle_gamma                 90.00
_cell_volume                   1630.46
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.16363 0.41195 0.34910
N2 N -0.12045 0.51016 0.38808
H*3 H -0.07047 0.48974 0.43013
N4 N -0.23008 0.43360 0.29306
H*5 H -0.24569 0.52580 0.28188
N6 N -0.14036 0.29210 0.36617
H*7 H -0.17472 0.22030 0.33529
N8 N -0.27417 0.32932 0.25317
N9 N -0.14605 0.63452 0.36913
H*10 H -0.13267 0.68309 0.27512
H*11 H -0.30120 0.33028 0.33669
H*12 H -0.30611 0.33297 0.11958
H*13 H -0.12777 0.68040 0.49223
N14 N -0.07068 0.27201 0.42499
H*15 H -0.05456 0.22113 0.54404
H*16 H -0.05947 0.22383 0.32693
C1 C 0.66669 -0.09598 0.14094
N2 N 0.62006 -0.18798 0.10641
H*3 H 0.57084 -0.16118 0.05557
N4 N 0.73233 -0.12616 0.20809
H*5 H 0.74466 -0.21985 0.23093
N6 N 0.64768 0.02620 0.10832
H*7 H 0.68457 0.09309 0.13632
N8 N 0.78008 -0.02824 0.24302
N9 N 0.64123 -0.31495 0.14168
H*10 H 0.62325 -0.36668 0.02354
H*11 H 0.80996 -0.02753 0.37861
H*12 H 0.80898 -0.04122 0.16584
H*13 H 0.62423 -0.35298 0.23631
N14 N 0.57876 0.05524 0.03813
H*15 H 0.56735 0.11311 0.12705
H*16 H 0.56637 0.09942 -0.08572
N'1+ N -0.06002 0.74905 -0.26816
N2+ N -0.08576 0.94479 -0.34514
```

```
N'3+ N -0.11130 0.82533 -0.35480
N'4+ N -0.00222 0.81441 -0.20268
C5+ C -0.01758 0.93759 -0.24998
C6+ C 0.03148 1.04188 -0.20480
N'7+ N 0.09806 1.02239 -0.10922
N'8+ N 0.12607 1.13825 -0.09540
N'9+ N 0.07868 1.22385 -0.17868
N'10+ N 0.01832 1.16610 -0.24929
O11+ O -0.12358 1.04188 -0.41773

#END

data_2TAGH_BTO_1_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                  20.086
_cell_length_b                  4.007
_cell_length_c                  10.981
_cell_angle_alpha                68.59
_cell_angle_beta                 78.84
_cell_angle_gamma                  90.05
_cell_volume                    804.774
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.39102 -0.27371 0.27396
N2 N 0.45926 -0.24717 0.24726
H*3 H 0.48365 -0.14931 0.14959
N4 N 0.35635 -0.40108 0.40109
H*5 H 0.38368 -0.47463 0.47435
N6 N 0.35745 -0.17288 0.17352
H*7 H 0.30574 -0.19719 0.19794
N8 N 0.28505 -0.42616 0.42635
N9 N 0.49314 -0.35434 0.35401
H*10 H 0.52278 -0.14254 0.34987
H*11 H 0.26664 -0.68672 0.47909
H*12 H 0.26676 -0.27133 0.47918
H*13 H 0.52267 -0.55792 0.34977
N14 N 0.39487 -0.04064 0.04152
H*15 H 0.38358 -0.19957 -0.00712
H*16 H 0.38370 0.21582 -0.00702
C1 C -0.09731 0.23099 0.76874
N2 N -0.02920 0.26726 0.73276
```

H*3 H -0.00812 0.36693 0.63332
N4 N -0.12771 0.10082 0.89858
H*5 H -0.09732 0.03275 0.96663
N6 N -0.13502 0.32489 0.67488
H*7 H -0.18649 0.29329 0.70626
N8 N -0.19897 0.06553 0.93359
N9 N 0.00907 0.16719 0.83277
H*10 H 0.03887 0.38335 0.82446
H*11 H -0.21561 -0.19680 0.98802
H*12 H -0.21560 0.21860 0.98810
H*13 H 0.03886 -0.03205 0.82438
N14 N -0.10203 0.46026 0.53986
H*15 H -0.11520 0.29872 0.49370
H*16 H -0.11519 0.71412 0.49377
N'1+ N 0.59728 0.17978 0.32046
N2+ N 0.68178 0.34769 0.15161
N'3+ N 0.61280 0.31149 0.18808
N'4+ N 0.65351 0.12914 0.37125
C5+ C 0.70704 0.23348 0.26633
C6+ C 0.77856 0.22207 0.27768
N'7+ N 0.79716 0.10247 0.39782
N'8+ N 0.86544 0.13237 0.36767
N'9+ N 0.88714 0.26386 0.23551
N'10+ N 0.83353 0.32352 0.17565
O11+ O 0.71312 0.47125 0.02741

#END

data_2TAGH_BTO_1_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 11.875
_cell_length_b 17.068
_cell_length_c 7.827
_cell_angle_alpha 90.00
_cell_angle_beta 84.68
_cell_angle_gamma 90.00
_cell_volume 1579.56
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

C1 C 0.68709 -0.30463 0.34091
N2 N 0.59949 -0.35377 0.37175
H*3 H 0.61519 -0.41213 0.35907
N4 N 0.67101 -0.22709 0.35578
H*5 H 0.59114 -0.20791 0.39071
N6 N 0.79078 -0.33303 0.29520
H*7 H 0.85494 -0.29385 0.27295
N8 N 0.76395 -0.17697 0.32285
N9 N 0.49196 -0.32262 0.41934
H*10 H 0.46246 -0.34284 0.53750
H*11 H 0.75077 -0.14030 0.22400
H*12 H 0.77560 -0.14498 0.42963
H*13 H 0.43762 -0.33816 0.33187
N14 N 0.80536 -0.41430 0.28055
H*15 H 0.83563 -0.42841 0.15841
H*16 H 0.86046 -0.43308 0.36404
C1 C 0.16471 0.82816 0.34302
N2 N 0.25611 0.87460 0.33439
H*3 H 0.24347 0.93281 0.35595
N4 N 0.17666 0.75094 0.31565
H*5 H 0.25642 0.72991 0.28873
N6 N 0.06136 0.85894 0.37902
H*7 H -0.00576 0.82176 0.38439
N8 N 0.07980 0.70366 0.32541
N9 N 0.36319 0.84100 0.29655
H*10 H 0.41185 0.85070 0.39498
H*11 H 0.07342 0.67659 0.21075
H*12 H 0.08389 0.66269 0.41921
H*13 H 0.40138 0.86460 0.18652
N14 N 0.05114 0.93982 0.40710
H*15 H 0.00363 0.96414 0.31910
H*16 H 0.01410 0.95024 0.52756
N'1+ N 0.47899 -0.07087 0.02184
N2+ N 0.53377 0.04892 0.03999
N'3+ N 0.44635 0.00255 0.00298
N'4+ N 0.58419 -0.07392 0.06964
C5+ C 0.61975 0.00093 0.08158
C6+ C 0.73111 0.02406 0.13071
N'7+ N 0.80944 -0.02938 0.16915
N'8+ N 0.89848 0.01350 0.20708
N'9+ N 0.87514 0.08930 0.19230
N'10+ N 0.77003 0.09802 0.14423
O11+ O 0.52815 0.12458 0.03323

#END

S62. Optimized crystal structure coordinates for 5 polymorphs of **9a** (ionic form).

data_2NH4_BTO_2_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id

```
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 8.092
_cell_length_b                 7.362
_cell_length_c                 8.636
_cell_angle_alpha               75.00
_cell_angle_beta               109.49
_cell_angle_gamma               60.39
_cell_volume                   360.953
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.72683 0.57893 -0.26487
H*2 H 0.75854 0.65371 -0.35743
H*3 H 0.60892 0.71352 -0.25560
H*4 H 0.66470 0.49970 -0.31511
H*5 H 0.87516 0.44879 -0.13135
N1 N 0.20899 0.60069 -0.34609
H*2 H 0.23941 0.68471 -0.43441
H*3 H 0.35877 0.46201 -0.21498
H*4 H 0.09467 0.72584 -0.32811
H*5 H 0.14311 0.53021 -0.40686
N'1+ N 0.41920 -0.12540 0.80862
N'2+ N 0.17084 0.19878 0.80837
N3+ N 0.26662 0.11818 0.71575
N'4+ N 0.42487 -0.21010 0.96993
C5+ C 0.27428 -0.01226 0.96713
C6+ C 0.22633 -0.02194 1.11786
N'7+ N 0.32797 -0.23068 1.27672
N'8+ N 0.23575 -0.15687 1.37380
N'9+ N 0.08527 0.08554 1.27766
N'10+ N 0.07532 0.17641 1.11515
O11+ O 0.21749 0.25984 0.55393

#END

data_2NH4_BTO_2_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                 8.408
_cell_length_b                 12.510
_cell_length_c                 4.135
```

```
_cell_angle_alpha               117.46
_cell_angle_beta                108.48
_cell_angle_gamma                87.28
_cell_volume                    363.506
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.26768 0.05736 0.14612
H*2 H -0.18384 0.12293 0.18520
H*3 H -0.34622 0.01536 -0.13667
H*4 H -0.20234 -0.00566 0.21115
H*5 H -0.33832 0.09680 0.32481
N1 N 0.24723 0.52781 0.04244
H*2 H 0.31814 0.45632 -0.00191
H*3 H 0.32575 0.60743 0.17649
H*4 H 0.16551 0.51640 -0.21886
H*5 H 0.17951 0.53109 0.21403
N'1+ N -0.02643 0.18934 1.09641
N'2+ N 0.13472 0.34524 1.19287
N3+ N 0.00317 0.30992 1.25222
N'4+ N 0.09064 0.14262 0.92622
C5+ C 0.18636 0.23786 0.98747
C6+ C 0.33033 0.22761 0.84906
N'7+ N 0.38322 0.12133 0.64425
N'8+ N 0.51579 0.15322 0.57887
N'9+ N 0.54158 0.27336 0.73728
N'10+ N 0.42641 0.32309 0.91037
O11+ O -0.08603 0.38405 1.43977

#END

data_2NH4_BTO_2_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                  14.984
_cell_length_b                  7.806
_cell_length_c                  4.084
_cell_angle_alpha                54.90
_cell_angle_beta                 68.43
_cell_angle_gamma                71.82
_cell_volume                    360.257
loop_
_atom_site_label
```

```
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.58674 0.19577 0.75069
H*2 H 0.59439 0.33821 0.69110
H*3 H 0.53298 0.21758 0.62552
H*4 H 0.65085 0.13483 0.62199
H*5 H 0.56874 0.09245 1.06415
N1 N 0.10798 0.68473 0.31502
H*2 H 0.07186 0.71058 0.11660
H*3 H 0.11762 0.82720 0.24883
H*4 H 0.06814 0.60378 0.61358
H*5 H 0.17430 0.59736 0.28107
N'1+ N 0.14795 0.02090 0.28362
N'2+ N 0.14796 0.33976 0.15808
N3+ N 0.10122 0.21677 0.16330
N'4+ N 0.22927 0.01365 0.36164
C5+ C 0.22793 0.20698 0.28429
C6+ C 0.30394 0.26855 0.33031
N'7+ N 0.38398 0.13808 0.45565
N'8+ N 0.43296 0.25648 0.45431
N'9+ N 0.38458 0.44966 0.33352
N'10+ N 0.30266 0.46242 0.25278
O11+ O 0.01967 0.27984 0.06310

#END

data_2NH4_BTO_2_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                 15.061
_cell_length_b                 7.078
_cell_length_c                 3.880
_cell_angle_alpha               100.34
_cell_angle_beta                115.92
_cell_angle_gamma                97.34
_cell_volume                   355.888
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.61643 -0.17959 0.50279
H*2 H 0.55173 -0.20053 0.53345
```

H*3 H 0.61476 -0.07556 0.34750
H*4 H 0.67899 -0.13166 0.77902
H*5 H 0.62024 -0.31060 0.35118
N1 N -0.09802 0.20031 0.91831
H*2 H -0.15745 0.16336 0.63463
H*3 H -0.03078 0.20931 0.90663
H*4 H -0.09782 0.33446 1.07348
H*5 H -0.10604 0.09411 1.05850
N'1+ N 0.67089 -0.85511 0.23461
N'2+ N 0.64577 -0.55117 0.22865
N3+ N 0.61064 -0.73243 0.24062
N'4+ N 0.74943 -0.75062 0.21793
C5+ C 0.73291 -0.56817 0.21460
C6+ C 0.80095 -0.40535 0.19773
N'7+ N 0.88796 -0.42006 0.18361
N'8+ N 0.92561 -0.24009 0.17127
N'9+ N 0.86399 -0.12224 0.17767
N'10+ N 0.78444 -0.22230 0.19437
O11+ O 0.52748 -0.78404 0.25630

#END

data_2NH4_BTO_2_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 13.804
_cell_length_b 7.076
_cell_length_c 3.883
_cell_angle_alpha 100.33
_cell_angle_beta 101.35
_cell_angle_gamma 100.92
_cell_volume 355.767
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.40186 -0.30005 0.51519
H*2 H 0.39388 -0.40601 0.66383
H*3 H 0.40175 -0.16583 0.66908
H*4 H 0.46929 -0.29077 0.43744
H*5 H 0.34252 -0.33759 0.29041
N1 N 0.11630 0.32048 0.38591
H*2 H 0.11408 0.42395 0.23128
H*3 H 0.05159 0.29884 0.48111

H*4 H 0.12061 0.18952 0.23177
H*5 H 0.17892 0.36961 0.59948
N'1+ N 0.17078 -0.35550 1.06240
N'2+ N 0.14585 -0.05119 1.08360
N3+ N 0.11069 -0.23261 1.13006
N'4+ N 0.24925 -0.25099 0.96686
C5+ C 0.23286 -0.06831 0.98128
C6+ C 0.30087 0.09461 0.89653
N'7+ N 0.38774 0.07977 0.79430
N'8+ N 0.42542 0.25990 0.74492
N'9+ N 0.36396 0.37796 0.81433
N'10+ N 0.28447 0.27788 0.91093
O11+ O 0.02762 -0.28418 1.22958

#END

S63. Optimized crystal structure coordinates for 5 polymorphs of **9b** (ionic form).

data_2NH3OH_BTO_2_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 17.226
_cell_length_b 11.524
_cell_length_c 4.338
_cell_angle_alpha 35.74
_cell_angle_beta 56.83
_cell_angle_gamma 69.93
_cell_volume 411.972
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.56456 -0.24978 0.87981
H*2 H 0.53150 -0.30294 0.86299
H*3 H 0.51924 -0.29936 1.26653
H*4 H 0.62637 -0.30366 0.88229
O5 O 0.58285 -0.03724 0.35249
H*6 H 0.61438 0.01949 0.35082
N1 N 0.09383 0.76046 0.35881
H*2 H 0.06042 0.69415 0.37879
H*3 H 0.05729 0.69424 0.77219
H*4 H 0.16277 0.73930 0.25621
O5 O 0.09012 0.96687 -0.10423
H*6 H 0.12124 1.03570 -0.13819
N'1+ N 0.16920 0.22740 -0.39809
N'2+ N 0.14287 0.47779 -0.57661

N3+ N 0.10685 0.33682 -0.40454
N'4+ N 0.25012 0.29893 -0.57359
C5+ C 0.23283 0.44948 -0.67888
C6+ C 0.30283 0.57002 -0.88121
N'7+ N 0.39267 0.54358 -0.98490
N'8+ N 0.43128 0.68308 -1.15936
N'9+ N 0.36753 0.78882 -1.16067
N'10+ N 0.28555 0.72104 -0.98692
O11+ O 0.02109 0.30890 -0.25977

#END

data_2NH3OH_BTO_2_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 8.373
_cell_length_b 13.272
_cell_length_c 10.311
_cell_angle_alpha 90.00
_cell_angle_beta 134.24
_cell_angle_gamma 90.00
_cell_volume 820.896
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.03207 0.98740 -0.15041
H*2 H 0.10730 0.98074 -0.19725
H*3 H 0.12940 0.95125 -0.02696
H*4 H 0.01550 1.06294 -0.13769
O5 O -0.17621 0.94026 -0.28345
H*6 H -0.25344 0.94493 -0.24404
N1 N 0.47907 0.27934 0.06930
H*2 H 0.32039 0.29180 0.01424
H*3 H 0.58353 0.33476 0.16390
H*4 H 0.53148 0.20890 0.12876
O5 O 0.45726 0.28485 -0.07863
H*6 H 0.60494 0.27338 -0.03201
N'1+ N -0.13796 0.22742 0.54280
N'2+ N 0.12047 0.21730 0.53377
N3+ N -0.04737 0.27099 0.48963
N'4+ N -0.02525 0.14103 0.62585

```
C5+ C 0.12949 0.13632 0.61901
C6+ C 0.29024 0.05339 0.69470
N'7+ N 0.30123 -0.02772 0.77993
N'8+ N 0.46862 -0.08366 0.82648
N'9+ N 0.55462 -0.03825 0.77171
N'10+ N 0.44550 0.04861 0.68790
O11+ O -0.11519 0.35586 0.40477

#END

data_2NH3OH_BTO_2_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                 8.349
_cell_length_b                 7.622
_cell_length_c                 13.774
_cell_angle_alpha               90.00
_cell_angle_beta                110.82
_cell_angle_gamma               90.00
_cell_volume                   819.288
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.24824 -0.06739 -0.28500
H*2 H -0.37119 -0.02148 -0.30143
H*3 H -0.20768 -0.12756 -0.21312
H*4 H -0.24815 -0.15505 -0.34218
O5 O -0.15113 0.08326 -0.28510
H*6 H -0.03295 0.04528 -0.26974
N1 N 0.34613 0.83818 -0.02002
H*2 H 0.22658 0.78276 -0.03742
H*3 H 0.33190 0.96395 -0.04984
H*4 H 0.40711 0.83983 0.05967
O5 O 0.43042 0.72822 -0.06846
H*6 H 0.54501 0.77642 -0.05379
N'1+ N -0.42212 -0.52222 0.78612
N'2+ N -0.16034 -0.53800 0.77752
N3+ N -0.32247 -0.48342 0.73151
N'4+ N -0.32166 -0.60624 0.87213
C5+ C -0.16468 -0.61441 0.86551
C6+ C -0.01466 -0.69633 0.94407
```

```
N'7+ N -0.01703 -0.77292 1.03205
N'8+ N 0.14429 -0.82960 1.08056
N'9+ N 0.23956 -0.78895 1.02428
N'10+ N 0.14284 -0.70459 0.93748
O11+ O -0.37742 -0.40192 0.64374

#END

data_2NH3OH_BTO_2_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                 19.979
_cell_length_b                 10.895
_cell_length_c                 4.038
_cell_angle_alpha               90.00
_cell_angle_beta                71.80
_cell_angle_gamma                 90.00
_cell_volume                   834.984
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.88378 0.44838 -0.03976
H*2 H 0.89455 0.53638 0.02237
H*3 H 0.84087 0.45076 -0.13072
H*4 H 0.92758 0.41398 -0.22762
O5 O 0.86898 0.38299 0.27511
H*6 H 0.85842 0.29854 0.22738
N1 N 0.35719 0.44138 0.52436
H*2 H 0.31797 0.43589 0.40904
H*3 H 0.38041 0.52697 0.47450
H*4 H 0.33526 0.42736 0.78930
O5 O 0.40464 0.34742 0.36608
H*6 H 0.44288 0.34945 0.46871
N'1+ N 0.24576 -0.36267 0.06878
N'2+ N 0.30317 -0.18471 0.03137
N3+ N 0.24727 -0.24320 -0.00990
N'4+ N 0.30319 -0.38438 0.16653
C5+ C 0.33703 -0.27618 0.14225
C6+ C 0.40302 -0.25833 0.22561
N'7+ N 0.43733 -0.34852 0.33628
N'8+ N 0.49403 -0.29308 0.38076
```

```
N'9+ N 0.49386 -0.17475 0.30044
N'10+ N 0.43699 -0.14983 0.20133
O11+ O 0.19972 -0.19029 -0.11447

#END

data_2NH3OH_BTO_2_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                 31.529
_cell_length_b                 6.911
_cell_length_c                 4.301
_cell_angle_alpha               90.00
_cell_angle_beta               123.14
_cell_angle_gamma                90.00
_cell_volume                   784.731
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.70384 -0.11199 0.93909
H*2 H 0.69646 0.01893 1.01492
H*3 H 0.73699 -0.10030 0.94566
H*4 H 0.70713 -0.21711 1.12179
O5 O 0.66177 -0.14473 0.57716
H*6 H 0.66729 -0.26825 0.49430
N1 N 0.05164 0.66957 0.57161
H*2 H 0.06003 0.79252 0.47976
H*3 H 0.03094 0.70834 0.68269
H*4 H 0.03120 0.57626 0.35022
O5 O 0.09908 0.59202 0.84241
H*6 H 0.09281 0.47447 0.93724
N'1+ N 0.05324 0.04449 0.34425
N'2+ N 0.08203 0.28379 0.15858
N3+ N 0.04723 0.22789 0.22762
N'4+ N 0.09380 -0.02429 0.35295
C5+ C 0.11058 0.12184 0.24031
C6+ C 0.15467 0.10885 0.20864
N'7+ N 0.18347 -0.05140 0.28902
N'8+ N 0.21899 -0.00069 0.22278
N'9+ N 0.21190 0.18197 0.10762
N'10+ N 0.17153 0.25535 0.09568
```

O11+ O 0.01159 0.33874 0.18641

#END

S64. Optimized crystal structure coordinates for 5 polymorphs of **9c** (ionic form).

```
data_2N2H5_BTO_2_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                 11.236
_cell_length_b                 11.677
_cell_length_c                 7.741
_cell_angle_alpha               90.00
_cell_angle_beta                58.24
_cell_angle_gamma                 90.00
_cell_volume                   863.559
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.50637 0.30869 -0.60264
H*2 H -0.40515 0.29310 -0.64124
H*3 H -0.54692 0.23149 -0.61158
N4 N -0.50192 0.38470 -0.75375
H*5 H -0.60268 0.39872 -0.71561
H*6 H -0.46010 0.46068 -0.74544
H*7 H -0.56316 0.33721 -0.45420
N1 N -0.08788 0.22362 0.92519
H*2 H -0.13971 0.14837 0.93868
H*3 H -0.13017 0.28486 0.87749
N4 N 0.05779 0.20872 0.76732
H*5 H 0.10816 0.28417 0.75331
H*6 H 0.09857 0.14690 0.81485
H*7 H -0.10724 0.24651 1.06662
N'1+ N -0.23937 0.39397 0.27995
N'2+ N -0.12827 0.55926 0.24307
N3+ N -0.24016 0.50764 0.25879
N'4+ N -0.12180 0.36909 0.27819
C5+ C -0.05641 0.46966 0.25587
C6+ C 0.07731 0.48184 0.24633
N'7+ N 0.15007 0.39343 0.25886
N'8+ N 0.26368 0.44209 0.24360
N'9+ N 0.25952 0.55480 0.22280
N'10+ N 0.14297 0.58268 0.22394
```

```
O11+ O -0.33864 0.56151 0.25410

#END

data_2N2H5_BTO_2_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                 15.242
_cell_length_b                 13.698
_cell_length_c                 4.148
_cell_angle_alpha               90.00
_cell_angle_beta                105.20
_cell_angle_gamma                90.00
_cell_volume                   835.743
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.44865 0.87268 0.56314
H*2 H 0.45996 0.81687 0.73507
H*3 H 0.44831 0.93635 0.69431
N4 N 0.35905 0.85948 0.33884
H*5 H 0.34795 0.91574 0.17134
H*6 H 0.35967 0.79559 0.21233
H*7 H 0.50205 0.87502 0.45311
N1 N 0.89906 0.14678 -0.47495
H*2 H 0.89659 0.08655 -0.32946
H*3 H 0.90169 0.20688 -0.32404
N4 N 0.81499 0.15096 -0.73711
H*5 H 0.81756 0.21152 -0.87810
H*6 H 0.81242 0.09050 -0.88355
H*7 H 0.95812 0.14394 -0.55241
N'1+ N 0.09680 0.04545 1.20144
N'2+ N 0.15581 0.17876 1.02933
N3+ N 0.08781 0.14133 1.14006
N'4+ N 0.17416 0.01807 1.12821
C5+ C 0.20864 0.09930 1.02513
C6+ C 0.29361 0.10229 0.91978
N'7+ N 0.34692 0.02379 0.91427
N'8+ N 0.41625 0.05863 0.80390
N'9+ N 0.40517 0.15388 0.74553
N'10+ N 0.32824 0.18374 0.81636
```

```
O11+ O 0.02056 0.19211 1.18338

#END

data_2N2H5_BTO_2_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                 4.097
_cell_length_b                 6.868
_cell_length_c                 30.968
_cell_angle_alpha               90.00
_cell_angle_beta                74.90
_cell_angle_gamma                 90.00
_cell_volume                   841.297
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.56938 0.29286 0.03762
H*2 H 0.70448 0.16667 0.03769
H*3 H 0.74339 0.40339 0.02873
N4 N 0.36938 0.32886 0.08285
H*5 H 0.23901 0.45547 0.08259
H*6 H 0.19987 0.21740 0.09160
H*7 H 0.43691 0.28135 0.01356
N1 N 0.48062 0.30824 0.21184
H*2 H 0.32982 0.18899 0.21130
H*3 H 0.33161 0.42919 0.21233
N4 N 0.74632 0.31056 0.17052
H*5 H 0.89260 0.43051 0.17109
H*6 H 0.89079 0.18894 0.17005
H*7 H 0.55861 0.30510 0.24097
N'1+ N -0.14324 0.55192 0.55698
N'2+ N -0.03478 0.82764 0.58891
N3+ N -0.12376 0.74621 0.55431
N'4+ N -0.06367 0.50229 0.59503
C5+ C 0.00074 0.67018 0.61375
C6+ C 0.09836 0.68289 0.65617
N'7+ N 0.13472 0.52741 0.68126
N'8+ N 0.22441 0.60367 0.71648
N'9+ N 0.24131 0.79652 0.71275
N'10+ N 0.16301 0.85123 0.67497
```

O11+ O -0.18458 0.84422 0.52174

#END

data_2N2H5_BTO_2_4
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P 1'
_symmetry_Int_Tables_number 1
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
_cell_length_a 10.012
_cell_length_b 6.780
_cell_length_c 4.219
_cell_angle_alpha 94.73
_cell_angle_beta 129.51
_cell_angle_gamma 72.92
_cell_volume 209.083
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.79858 0.62609 -0.00239
H*2 H 0.90153 0.55746 -0.01362
H*3 H 0.77007 0.50693 0.05733
N4 N 0.63844 0.73931 -0.40896
H*5 H 0.53633 0.80501 -0.39646
H*6 H 0.66854 0.85582 -0.46782
H*7 H 0.84552 0.71242 0.24107
N1 N 0.10010 -0.04775 0.22027
H*2 H 0.06242 -0.14356 -0.00585
H*3 H 0.10887 0.07809 0.12158
N4 N 0.28017 -0.15915 0.59649
H*5 H 0.31740 -0.06218 0.81798
H*6 H 0.27069 -0.28510 0.68982
H*7 H -0.00116 0.00414 0.24252
N'1+ N 0.19186 0.26773 0.06904
N'2+ N 0.29264 0.48249 -0.04727
N3+ N 0.16141 0.46299 -0.05418
N'4+ N 0.35025 0.15266 0.16175
C5+ C 0.40872 0.28468 0.08975
C6+ C 0.57838 0.22316 0.15147
N'7+ N 0.69529 0.02684 0.28771
N'8+ N 0.82952 0.04021 0.29877
N'9+ N 0.79496 0.23588 0.17471
N'10+ N 0.63712 0.35548 0.07932
O11+ O 0.02020 0.61597 -0.16751

#END

```
data_2N2H5_BTO_2_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                 27.687
_cell_length_b                 4.901
_cell_length_c                 6.447
_cell_angle_alpha               90.00
_cell_angle_beta                91.12
_cell_angle_gamma                 90.00
_cell_volume                   874.652
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.71100 -0.98951 0.34298
H*2 H 0.71257 -1.07375 0.48910
H*3 H 0.74542 -0.99840 0.28611
N4 N 0.69773 -0.70505 0.36300
H*5 H 0.69678 -0.62219 0.21756
H*6 H 0.66374 -0.69797 0.42170
H*7 H 0.68852 -1.10749 0.24996
N1 N -0.05484 0.25317 0.77808
H*2 H -0.03131 0.14778 0.87408
H*3 H -0.06369 0.12441 0.65719
N4 N -0.02936 0.48537 0.69459
H*5 H -0.05279 0.58713 0.59769
H*6 H -0.02023 0.61062 0.81581
H*7 H -0.08575 0.29668 0.85888
N'1+ N 0.07532 0.06017 -0.41474
N'2+ N 0.07824 0.25517 -0.10157
N3+ N 0.05660 0.07010 -0.22511
N'4+ N 0.11094 0.24687 -0.41708
C5+ C 0.11213 0.36196 -0.22727
C6+ C 0.14606 0.57827 -0.16232
N'7+ N 0.17999 0.68661 -0.28574
N'8+ N 0.20258 0.87415 -0.16657
N'9+ N 0.18311 0.87856 0.02032
N'10+ N 0.14727 0.69382 0.02803
O11+ O 0.02138 -0.08302 -0.16798

#END
```

S65. Optimized crystal structure coordinates for 5 polymorphs of **9d** (ionic form).

```
data_2GH_BTO_2_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                 3.546
_cell_length_b                 29.039
_cell_length_c                 10.702
_cell_angle_alpha               90.00
_cell_angle_beta                77.32
_cell_angle_gamma                 90.00
_cell_volume                   1075.13
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.43820 0.46309 0.46180
N2 N 0.53738 0.47758 0.34039
H*3 H 0.69409 0.45752 0.27081
H*4 H 0.45850 0.50902 0.31468
N5 N 0.54659 0.42131 0.49309
H*6 H 0.47476 0.40968 0.58423
H*7 H 0.70349 0.40014 0.42650
N8 N 0.23064 0.49038 0.55192
H*9 H 0.14575 0.52207 0.53036
H*10 H 0.15262 0.48011 0.64422
C1 C 0.17932 0.28381 0.58652
N2 N 0.23651 0.27805 0.70495
H*3 H 0.31570 0.24720 0.73464
H*4 H 0.20222 0.30437 0.76821
N5 N 0.22682 0.24836 0.50480
H*6 H 0.18510 0.25196 0.41489
H*7 H 0.30582 0.21693 0.53056
N8 N 0.07463 0.32502 0.54982
H*9 H 0.03716 0.35227 0.61004
H*10 H 0.02993 0.33013 0.46079
N'1+ N -0.50704 0.12063 0.77561
N'2+ N -0.47951 0.16756 0.60848
N3+ N -0.50803 0.16422 0.73515
N'4+ N -0.47653 0.09388 0.67118
C5+ C -0.46035 0.12276 0.57162
C6+ C -0.42593 0.10783 0.43818
N'7+ N -0.40655 0.06335 0.40003
```

N'8+ N -0.37757 0.06531 0.27277
N'9+ N -0.37942 0.10903 0.23592
N'10+ N -0.40968 0.13677 0.33826
O11+ O -0.53381 0.19925 0.81064

#END

data_2GH_BTO_2_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 9.175
_cell_length_b 16.602
_cell_length_c 7.103
_cell_angle_alpha 90.00
_cell_angle_beta 97.85
_cell_angle_gamma 90.00
_cell_volume 1071.81
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.41698 0.16433 0.45682
N2 N 0.44138 0.09060 0.53025
H*3 H 0.36265 0.04765 0.51283
H*4 H 0.53927 0.07569 0.60530
N5 N 0.28635 0.18239 0.35810
H*6 H 0.26559 0.23772 0.30141
H*7 H 0.20457 0.14123 0.33731
N8 N 0.52321 0.22000 0.48211
H*9 H 0.62270 0.20762 0.55622
H*10 H 0.50710 0.27607 0.42785
C1 C 0.12635 0.65383 0.04760
N2 N 0.26075 0.66592 0.14254
H*3 H 0.33567 0.62100 0.16129
H*4 H 0.29133 0.72033 0.19830
N5 N 0.08887 0.58118 -0.02469
H*6 H -0.01208 0.57074 -0.09690
H*7 H 0.16042 0.53459 -0.00921
N8 N 0.02942 0.71439 0.02495
H*9 H 0.05547 0.76975 0.07841
H*10 H -0.07270 0.70656 -0.04629
N'1+ N -0.26732 0.04894 0.66312

N'2+ N -0.03577 0.08342 0.77196
N3+ N -0.17494 0.10851 0.72552
N'4+ N -0.18584 -0.01864 0.66840
C5+ C -0.04687 0.00337 0.73427
C6+ C 0.07892 -0.05239 0.76253
N'7+ N 0.06956 -0.13224 0.72564
N'8+ N 0.20780 -0.15966 0.77073
N'9+ N 0.29647 -0.09903 0.83205
N'10+ N 0.21835 -0.03037 0.82859
O11+ O -0.21614 0.18231 0.73926

#END

data_2GH_BTO_2_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 3.577
_cell_length_b 33.319
_cell_length_c 9.073
_cell_angle_alpha 90.00
_cell_angle_beta 94.47
_cell_angle_gamma 90.00
_cell_volume 1078.05
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.59098 0.29993 0.41459
N2 N 0.65718 0.29319 0.27367
H*3 H 0.59485 0.31398 0.19444
H*4 H 0.77148 0.26711 0.24230
N5 N 0.43944 0.33472 0.45296
H*6 H 0.38710 0.34043 0.55879
H*7 H 0.37283 0.35633 0.37724
N8 N 0.67632 0.27187 0.51714
H*9 H 0.79099 0.24538 0.49054
H*10 H 0.62863 0.27635 0.62423
C1 C 0.54702 0.04404 0.11171
N2 N 0.74603 0.03513 0.23839
H*3 H 0.84279 0.00705 0.25943
H*4 H 0.80546 0.05622 0.31678
N5 N 0.47254 0.01552 0.00992

H*6 H 0.32269 0.02160 -0.08654
H*7 H 0.56394 -0.01294 0.02648
N8 N 0.42249 0.08146 0.08682
H*9 H 0.47558 0.10346 0.16224
H*10 H 0.27165 0.08884 -0.00813
N'1+ N -0.16210 0.15296 0.25172
N'2+ N -0.00565 0.16821 0.48825
N3+ N -0.06469 0.18192 0.34946
N'4+ N -0.16792 0.11854 0.32908
C5+ C -0.07302 0.12835 0.47114
C6+ C -0.04492 0.09944 0.59415
N'7+ N -0.11115 0.05966 0.57881
N'8+ N -0.05441 0.04479 0.71649
N'9+ N 0.04172 0.07431 0.81055
N'10+ N 0.05025 0.10925 0.73667
O11+ O -0.03149 0.21911 0.31326

#END

data_2GH_BTO_2_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 18.427
_cell_length_b 8.261
_cell_length_c 7.403
_cell_angle_alpha 90.00
_cell_angle_beta 74.72
_cell_angle_gamma 90.00
_cell_volume 1087.09
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.84669 -0.36423 0.56884
N2 N 0.91954 -0.39209 0.55375
H*3 H 0.93640 -0.48989 0.61401
H*4 H 0.95986 -0.31616 0.48166
N5 N 0.79453 -0.46679 0.66513
H*6 H 0.73919 -0.44802 0.67826
H*7 H 0.80895 -0.56605 0.72756
N8 N 0.82599 -0.23381 0.48764
H*9 H 0.86448 -0.15477 0.41425

H*10 H 0.77126 -0.21047 0.49730
C1 C 0.33567 0.89473 0.10019
N2 N 0.40858 0.91990 0.08703
H*3 H 0.42632 1.02202 0.13730
H*4 H 0.44805 0.83754 0.02643
N5 N 0.28465 1.00584 0.18111
H*6 H 0.22928 0.98925 0.19251
H*7 H 0.29997 1.10965 0.23322
N8 N 0.31379 0.75844 0.03243
H*9 H 0.35140 0.67292 -0.02924
H*10 H 0.25899 0.73700 0.04091
N'1+ N 0.44608 -0.77851 0.20726
N'2+ N 0.42176 -0.52805 0.32078
N3+ N 0.39361 -0.67407 0.29832
N'4+ N 0.51194 -0.69824 0.16757
C5+ C 0.49612 -0.54779 0.23701
C6+ C 0.55247 -0.41906 0.22425
N'7+ N 0.62670 -0.43692 0.14128
N'8+ N 0.65701 -0.29213 0.16108
N'9+ N 0.60341 -0.19154 0.25193
N'10+ N 0.53665 -0.26813 0.29386
O11+ O 0.32330 -0.71076 0.35799

#END

data_2GH_BTO_2_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 29.459
_cell_length_b 3.546
_cell_length_c 10.342
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1080.34
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.21570 0.77390 -0.04713
N2 N 0.17583 0.90442 -0.00447
H*3 H 0.15094 0.97988 -0.06653

H*4 H 0.16943 0.93141 0.09108
N5 N 0.22324 0.74114 -0.17415
H*6 H 0.25312 0.64317 -0.20845
H*7 H 0.19928 0.81340 -0.23954
N8 N 0.24803 0.67613 0.03722
H*9 H 0.24304 0.69865 0.13359
H*10 H 0.27840 0.57689 0.00706
C1 C 0.04003 0.34297 0.09815
N2 N 0.08279 0.43071 0.06680
H*3 H 0.09513 0.37973 -0.02268
H*4 H 0.10400 0.55054 0.13167
N5 N 0.01270 0.18457 0.01033
H*6 H -0.01971 0.11604 0.03198
H*7 H 0.02368 0.12877 -0.08025
N8 N 0.02460 0.41363 0.21732
H*9 H 0.04467 0.53314 0.28514
H*10 H -0.00759 0.34960 0.24303
N'1+ N 0.37786 0.27884 -0.21471
N'2+ N 0.33328 0.42280 -0.04710
N3+ N 0.33549 0.34389 -0.17372
N'4+ N 0.40493 0.31624 -0.11070
C5+ C 0.37748 0.40286 -0.01085
C6+ C 0.39323 0.46868 0.12230
N'7+ N 0.43712 0.44982 0.15984
N'8+ N 0.43627 0.52778 0.28703
N'9+ N 0.39376 0.59079 0.32442
N'10+ N 0.36572 0.55558 0.22251
O11+ O 0.30054 0.33157 -0.24871

#END

S66. Optimized crystal structure coordinates for 5 polymorphs of **9e** (ionic form).

data_2AGH_BTO_2_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a 13.443
_cell_length_b 12.557
_cell_length_c 8.094
_cell_angle_alpha 90.00
_cell_angle_beta 75.77
_cell_angle_gamma 90.00
_cell_volume 1324.38
loop_
_atom_site_label
_atom_site_type_symbol

```
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.70575 0.77432 -0.36444
N2 N 0.62305 0.71921 -0.28203
H*3 H 0.62978 0.64695 -0.23095
H*4 H 0.55153 0.74850 -0.26869
N5 N 0.79976 0.73246 -0.37944
H*6 H 0.80705 0.65991 -0.32843
N7 N 0.69680 0.86941 -0.43161
H*8 H 0.62764 0.90340 -0.42298
H*9 H 0.76188 0.90774 -0.49267
N10 N 0.88586 0.79040 -0.46567
H*11 H 0.93185 0.80689 -0.38595
H*12 H 0.92565 0.74884 -0.56895
C1 C 0.78286 0.07638 -0.17971
N2 N 0.86897 0.13261 -0.23886
H*3 H 0.86666 0.20908 -0.27656
H*4 H 0.93873 0.09997 -0.24740
N5 N 0.69137 0.12284 -0.17036
H*6 H 0.68852 0.19963 -0.20802
N7 N 0.78598 -0.02426 -0.13014
H*8 H 0.85310 -0.06180 -0.13525
H*9 H 0.71853 -0.06317 -0.08638
N10 N 0.60169 0.06371 -0.10847
H*11 H 0.55765 0.09851 -0.00164
H*12 H 0.56145 0.05742 -0.19949
N'1+ N 0.06224 0.48507 0.25271
N'2+ N 0.13807 0.64135 0.27160
N3+ N 0.05004 0.59032 0.27455
N'4+ N 0.16277 0.46543 0.23448
C5+ C 0.20706 0.56045 0.24622
C6+ C 0.31729 0.57560 0.23323
N'7+ N 0.38691 0.49583 0.20798
N'8+ N 0.47667 0.54417 0.20427
N'9+ N 0.46176 0.64842 0.22630
N'10+ N 0.36178 0.67088 0.24499
O11+ O -0.03751 0.63736 0.29613

#END

data_2AGH_BTO_2_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                 10.584
_cell_length_b                 11.262
_cell_length_c                 10.999
_cell_angle_alpha               90.00
_cell_angle_beta                77.36
_cell_angle_gamma                 90.00
_cell_volume                   1279.27
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.36837 0.03842 0.10346
N2 N 0.29420 -0.05207 0.08163
H*3 H 0.23773 -0.04509 0.01884
H*4 H 0.29271 -0.12995 0.12747
N5 N 0.36758 0.14078 0.04036
H*6 H 0.31108 0.14837 -0.02283
N7 N 0.44265 0.02914 0.18611
H*8 H 0.44583 -0.04614 0.23521
H*9 H 0.49692 0.10033 0.19904
N10 N 0.44527 0.23499 0.06357
H*11 H 0.51112 0.25674 -0.01554
H*12 H 0.38938 0.30669 0.09615
C1 C 0.14838 0.13893 0.38165
N2 N 0.19260 0.04561 0.43547
H*3 H 0.26003 0.05537 0.48706
H*4 H 0.15962 -0.03727 0.42588
N5 N 0.19485 0.24798 0.39671
H*6 H 0.26259 0.25838 0.44843
N7 N 0.05963 0.12599 0.31377
H*8 H 0.02250 0.04568 0.30037
H*9 H 0.02950 0.19958 0.27510
N10 N 0.14829 0.34512 0.34028
H*11 H 0.10481 0.40450 0.40612
H*12 H 0.22200 0.38485 0.27860
N'1+ N 0.81026 -0.15088 0.12033
N'2+ N 0.92707 -0.06027 0.23930
N3+ N 0.84839 -0.04725 0.15984
N'4+ N 0.86611 -0.23640 0.17604
C5+ C 0.93598 -0.18009 0.24722
C6+ C 1.01323 -0.24061 0.32479
N'7+ N 1.02302 -0.35982 0.33361
N'8+ N 1.10164 -0.37645 0.41298
N'9+ N 1.13760 -0.27189 0.45029
N'10+ N 1.08333 -0.18419 0.39621
O11+ O 0.81281 0.05437 0.12479

#END

data_2AGH_BTO_2_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                 10.270
_cell_length_b                 16.857
_cell_length_c                 11.309
_cell_angle_alpha               90.00
_cell_angle_beta               139.53
_cell_angle_gamma                90.00
_cell_volume                   1270.73
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.27252 0.16249 0.43059
N2 N 0.25913 0.20759 0.51857
H*3 H 0.25836 0.26743 0.51303
H*4 H 0.24940 0.18291 0.59304
N5 N 0.28522 0.19772 0.33276
H*6 H 0.28454 0.25780 0.32664
N7 N 0.27351 0.08374 0.43797
H*8 H 0.26425 0.05519 0.50987
H*9 H 0.28393 0.05242 0.36884
N10 N 0.29918 0.15030 0.24115
H*11 H 0.18013 0.16048 0.10451
H*12 H 0.43014 0.16139 0.28826
C1 C 0.76888 0.11623 -0.08316
N2 N 0.73111 0.16511 -0.01853
H*3 H 0.71529 0.22416 -0.04167
H*4 H 0.71739 0.14420 0.05531
N5 N 0.78609 0.14649 -0.18100
H*6 H 0.77036 0.20574 -0.20474
N7 N 0.78968 0.03854 -0.05263
H*8 H 0.77780 0.01366 0.02010
H*9 H 0.81816 0.00421 -0.10467
N10 N 0.82555 0.09513 -0.24816
H*11 H 0.71189 0.09741 -0.38679
H*12 H 0.95813 0.10968 -0.19574
N'1+ N 0.24423 0.36545 0.28219
N'2+ N 0.21645 0.48217 0.35508
N3+ N 0.21488 0.40296 0.36475
N'4+ N 0.26622 0.42227 0.21481
C5+ C 0.24903 0.49206 0.26009
```

```
C6+ C 0.26363 0.57019 0.21272
N'7+ N 0.29602 0.58097 0.11821
N'8+ N 0.29857 0.66014 0.10569
N'9+ N 0.26903 0.69547 0.18896
N'10+ N 0.24640 0.64023 0.25808
O11+ O 0.18797 0.36640 0.44508

#END

data_2AGH_BTO_2_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                 7.394
_cell_length_b                 16.597
_cell_length_c                 11.063
_cell_angle_alpha               90.00
_cell_angle_beta                104.76
_cell_angle_gamma                90.00
_cell_volume                   1312.83
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.68831 0.27243 0.39534
N2 N 0.76613 0.22546 0.49328
H*3 H 0.79418 0.16676 0.48204
H*4 H 0.79896 0.24754 0.58127
N5 N 0.64667 0.24067 0.27953
H*6 H 0.67449 0.18175 0.26760
N7 N 0.65146 0.34968 0.41023
H*8 H 0.68067 0.37564 0.49556
H*9 H 0.59248 0.38252 0.33294
N10 N 0.56540 0.29002 0.17758
H*11 H 0.64975 0.29337 0.11792
H*12 H 0.43717 0.26840 0.13215
C1 C 0.70771 0.03761 -0.12122
N2 N 0.73694 0.08083 -0.01572
H*3 H 0.74230 0.14164 -0.01701
H*4 H 0.75446 0.05370 0.06821
N5 N 0.68502 0.07608 -0.23123
H*6 H 0.69025 0.13716 -0.23317
N7 N 0.70068 -0.04243 -0.11943
```

H*8 H 0.71705 -0.07340 -0.03880
H*9 H 0.67819 -0.07221 -0.20197
N10 N 0.65453 0.03061 -0.34112
H*11 H 0.52824 0.04474 -0.39957
H*12 H 0.75881 0.04058 -0.38429
N'1+ N 0.22439 0.25314 0.79184
N'2+ N 0.24177 0.13560 0.89252
N3+ N 0.23580 0.21609 0.90095
N'4+ N 0.22273 0.19465 0.70733
C5+ C 0.23329 0.12439 0.76972
C6+ C 0.23547 0.04452 0.71230
N'7+ N 0.22711 0.03241 0.59018
N'8+ N 0.23280 -0.04808 0.57803
N'9+ N 0.24409 -0.08290 0.68795
N'10+ N 0.24606 -0.02599 0.77482
O11+ O 0.24050 0.25419 1.00332

#END

data_2AGH_BTO_2_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 7.302
_cell_length_b 16.855
_cell_length_c 11.419
_cell_angle_alpha 90.00
_cell_angle_beta 63.41
_cell_angle_gamma 90.00
_cell_volume 1256.75
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.47239 0.11050 0.49747
N2 N 0.43685 0.06484 0.41377
H*3 H 0.42047 0.00544 0.42584
H*4 H 0.42543 0.08863 0.33612
N5 N 0.48655 0.07646 0.59978
H*6 H 0.47025 0.01683 0.61246
N7 N 0.49391 0.18866 0.48151
H*8 H 0.48429 0.21633 0.40602
H*9 H 0.52061 0.22044 0.54771

N10 N 0.52369 0.12446 0.68688
H*11 H 0.40579 0.12008 0.77867
H*12 H 0.65782 0.10857 0.68753
C1 C -0.03865 -0.11354 0.82095
N2 N -0.02049 -0.06642 0.90968
H*3 H -0.01447 -0.00676 0.89993
H*4 H -0.01231 -0.08932 0.98894
N5 N -0.04908 -0.08065 0.71665
H*6 H -0.04312 -0.02077 0.70628
N7 N -0.04656 -0.19203 0.83387
H*8 H -0.03919 -0.21887 0.91071
H*9 H -0.06035 -0.22494 0.76388
N10 N -0.06804 -0.13017 0.62430
H*11 H -0.20091 -0.11833 0.61899
H*12 H 0.05402 -0.12288 0.53488
N'1+ N 0.45426 0.09261 0.11713
N'2+ N 0.41189 0.21044 0.04305
N3+ N 0.41403 0.13142 0.02905
N'4+ N 0.47993 0.14834 0.19288
C5+ C 0.45384 0.21882 0.14675
C6+ C 0.46875 0.29617 0.20168
N'7+ N 0.51041 0.30545 0.30489
N'8+ N 0.50956 0.38438 0.32201
N'9+ N 0.46919 0.42102 0.23305
N'10+ N 0.44260 0.36689 0.15547
O11+ O 0.38087 0.09615 -0.05988

#END

S67. Optimized crystal structure coordinates for 5 polymorphs of **9f** (ionic form).

data_2DAGH_BTO_2_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 16.039
_cell_length_b 12.345
_cell_length_c 7.532
_cell_angle_alpha 90.00
_cell_angle_beta 105.24
_cell_angle_gamma 90.00
_cell_volume 1438.9
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y

```
_atom_site_fract_z
C1 C 0.43352 0.62284 0.25347
N2 N 0.35905 0.62942 0.12197
H*3 H 0.30432 0.64424 0.16190
N4 N 0.43282 0.63595 0.43074
H*5 H 0.48892 0.63111 0.53132
N6 N 0.50731 0.60355 0.20923
H*7 H 0.50477 0.59423 0.07416
H*8 H 0.56434 0.59819 0.30558
N9 N 0.35411 0.65611 0.47224
N10 N 0.36019 0.61571 -0.06209
H*11 H 0.33766 0.68388 -0.13516
H*12 H 0.34097 0.59614 0.55368
H*13 H 0.35591 0.72915 0.53591
H*14 H 0.32275 0.55119 -0.11744
C1 C -0.47127 0.11410 0.91235
N2 N -0.40728 0.06842 0.85487
H*3 H -0.41840 0.05235 0.71825
N4 N -0.54667 0.13653 0.78845
H*5 H -0.59553 0.17113 0.83070
N6 N -0.46036 0.13699 1.08989
H*7 H -0.40258 0.11870 1.17817
H*8 H -0.50751 0.17141 1.13692
N9 N -0.55589 0.11138 0.60299
N10 N -0.32903 0.04528 0.98433
H*11 H -0.27997 0.08664 0.95240
H*12 H -0.60471 0.05714 0.55817
H*13 H -0.56763 0.17982 0.52495
H*14 H -0.31697 -0.03575 0.98554
N'1+ N 0.58729 0.74846 -0.20421
N'2+ N 0.72924 0.72824 -0.16716
N3+ N 0.66678 0.76973 -0.09917
N'4+ N 0.59745 0.69032 -0.34821
C5+ C 0.68330 0.67902 -0.32339
C6+ C 0.72323 0.62034 -0.45005
N'7+ N 0.67834 0.57094 -0.60611
N'8+ N 0.73912 0.52813 -0.67859
N'9+ N 0.81715 0.55075 -0.57096
N'10+ N 0.80933 0.60897 -0.42526
O11+ O 0.68143 0.82450 0.05172

#END

data_2DAGH_BTO_2_2
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P c'
_symmetry_Int_Tables_number      7
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 x,-y,1/2+z
```

```
_cell_length_a                 7.389
_cell_length_b                 7.447
_cell_length_c                 13.408
_cell_angle_alpha               90.00
_cell_angle_beta                80.06
_cell_angle_gamma               90.00
_cell_volume                   726.712
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.31892 0.25291 -0.16482
N2 N 0.16302 0.32817 -0.11741
H*3 H 0.06032 0.24488 -0.08525
N4 N 0.33298 0.07247 -0.16789
H*5 H 0.45055 0.01423 -0.20363
N6 N 0.45820 0.35545 -0.20836
H*7 H 0.44152 0.49054 -0.20417
H*8 H 0.57721 0.30224 -0.24458
N9 N 0.18391 -0.03115 -0.12133
N10 N 0.14921 0.51585 -0.11447
H*11 H 0.12715 0.55888 -0.04128
H*12 H 0.13743 -0.11051 -0.17336
H*13 H 0.22101 -0.10790 -0.06534
H*14 H 0.04377 0.55627 -0.14904
C1 C 0.43150 -0.19721 0.57272
N2 N 0.59056 -0.26694 0.52572
H*3 H 0.69139 -0.18005 0.49553
N4 N 0.41199 -0.01733 0.57796
H*5 H 0.29199 0.03673 0.61341
N6 N 0.29445 -0.30464 0.61373
H*7 H 0.31524 -0.43909 0.60797
H*8 H 0.17315 -0.25565 0.64958
N9 N 0.55886 0.09151 0.53404
N10 N 0.61003 -0.45407 0.52051
H*11 H 0.71527 -0.49295 0.55567
H*12 H 0.52130 0.16913 0.47852
H*13 H 0.60121 0.17028 0.58766
H*14 H 0.63554 -0.49410 0.44679
N'1+ N 0.87693 -0.30123 -0.20836
N'2+ N 0.68477 -0.07799 -0.22883
N3+ N 0.70386 -0.24082 -0.18926
N'4+ N 0.97705 -0.17284 -0.26299
C5+ C 0.85895 -0.03968 -0.27449
C6+ C 0.91134 0.12820 -0.32995
N'7+ N 1.08420 0.16823 -0.37580
N'8+ N 1.07052 0.33153 -0.41659
N'9+ N 0.89712 0.38736 -0.39621
N'10+ N 0.79298 0.26183 -0.34152
O11+ O 0.56983 -0.33052 -0.13805
```

```
#END

data_2DAGH_BTO_2_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                 13.888
_cell_length_b                 6.415
_cell_length_c                 15.611
_cell_angle_alpha               90.00
_cell_angle_beta                74.32
_cell_angle_gamma                 90.00
_cell_volume                   1339.05
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.47277 -0.24279 0.51277
N2 N 0.45648 -0.23095 0.43221
H*3 H 0.38519 -0.20501 0.42938
N4 N 0.39509 -0.22015 0.58569
H*5 H 0.40670 -0.22888 0.64700
N6 N 0.56470 -0.27656 0.52056
H*7 H 0.62085 -0.29264 0.46391
H*8 H 0.57907 -0.28618 0.58045
N9 N 0.29950 -0.18485 0.57504
N10 N 0.53753 -0.25462 0.35665
H*11 H 0.54598 -0.12322 0.31873
H*12 H 0.25226 -0.30188 0.60382
H*13 H 0.27254 -0.04518 0.60215
H*14 H 0.52574 -0.37932 0.32040
C1 C 0.77525 0.31651 -0.01721
N2 N 0.79712 0.30553 0.06110
H*3 H 0.87049 0.29753 0.06020
N4 N 0.85035 0.31651 -0.09287
H*5 H 0.83452 0.32478 -0.15251
N6 N 0.68037 0.32730 -0.02011
H*7 H 0.62632 0.32685 0.03844
H*8 H 0.66179 0.33571 -0.07822
N9 N 0.94918 0.30500 -0.08734
N10 N 0.71872 0.30560 0.13953
H*11 H 0.72531 0.43077 0.17767
```

H*12 H 0.98297 0.17430 -0.11851
H*13 H 0.98800 0.43411 -0.11491
H*14 H 0.72029 0.17157 0.17408
N'1+ N -0.24580 0.75993 0.35294
N'2+ N -0.18572 0.65059 0.21277
N3+ N -0.24101 0.79319 0.26727
N'4+ N -0.19129 0.58769 0.35536
C5+ C -0.15578 0.52427 0.27038
C6+ C -0.09195 0.33983 0.24259
N'7+ N -0.06153 0.21259 0.29919
N'8+ N -0.00556 0.06673 0.24668
N'9+ N -0.00241 0.10446 0.16221
N'10+ N -0.05630 0.27610 0.15737
O11+ O -0.28516 0.94680 0.24032

#END

data_2DAGH_BTO_2_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 10.645
_cell_length_b 7.456
_cell_length_c 20.106
_cell_angle_alpha 114.40
_cell_angle_beta 83.03
_cell_angle_gamma 42.58
_cell_volume 711.172
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.70204 0.58645 -0.11204
N2 N -0.62595 0.63191 -0.07083
H*3 H -0.58031 0.53784 -0.04024
N4 N -0.71477 0.42028 -0.11124
H*5 H -0.77220 0.38462 -0.14227
N6 N -0.76428 0.70430 -0.15326
H*7 H -0.75185 0.82773 -0.15215
H*8 H -0.82223 0.67356 -0.18482
N9 N -0.64795 0.29987 -0.06728
N10 N -0.61309 0.80487 -0.07189
H*11 H -0.42987 0.60840 -0.11080
H*12 H -0.80046 0.45208 -0.00834
H*13 H -0.49629 0.00047 -0.11956

H*14 H -0.73334 1.05896 0.00015
C1 C 0.28359 -0.39202 0.37080
N2 N 0.35571 -0.33489 0.41170
H*3 H 0.39629 -0.41412 0.44573
N4 N 0.26804 -0.54989 0.37637
H*5 H 0.21358 -0.59427 0.34560
N6 N 0.22801 -0.29374 0.32520
H*7 H 0.24234 -0.17591 0.32281
H*8 H 0.17318 -0.33362 0.29375
N9 N 0.32785 -0.64968 0.42484
N10 N 0.37152 -0.17064 0.40567
H*11 H 0.55441 -0.36615 0.36723
H*12 H 0.17265 -0.48957 0.48507
H*13 H 0.47902 -0.94763 0.37565
H*14 H 0.24876 0.09084 0.47639
N'1+ N 0.82328 0.46085 0.32925
N'2+ N 1.02892 0.47112 0.31746
N3+ N 0.93824 0.44436 0.35585
N'4+ N 0.83837 0.50028 0.27064
C5+ C 0.96273 0.50585 0.26446
C6+ C 1.02092 0.54491 0.20714
N'7+ N 0.95624 0.57975 0.15401
N'8+ N 1.04451 0.60746 0.11416
N'9+ N 1.15733 0.59008 0.14205
N'10+ N 1.14565 0.55053 0.20090
O11+ O 0.95908 0.40662 0.41257

#END

data_2DAGH_BTO_2_5
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 8.135
_cell_length_b 7.173
_cell_length_c 12.364
_cell_angle_alpha 91.84
_cell_angle_beta 89.24
_cell_angle_gamma 82.42
_cell_volume 714.684
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.30402 0.46384 0.55738

N2 N 0.32295 0.31268 0.48977
H*3 H 0.41130 0.20450 0.50730
N4 N 0.40150 0.46623 0.64459
H*5 H 0.38807 0.58013 0.69626
N6 N 0.19015 0.60988 0.53847
H*7 H 0.11962 0.60193 0.47190
H*8 H 0.17328 0.72555 0.58810
N9 N 0.51987 0.31032 0.66195
N10 N 0.22124 0.31102 0.39923
H*11 H 0.15327 0.20180 0.40271
H*12 H 0.63594 0.34880 0.66112
H*13 H 0.49669 0.25236 0.73376
H*14 H 0.29219 0.29802 0.33024
C1 C 0.17999 0.56158 -0.04975
N2 N 0.16067 0.72001 0.01197
H*3 H 0.07655 0.82799 -0.01166
N4 N 0.08844 0.55202 -0.13934
H*5 H 0.10221 0.43259 -0.18660
N6 N 0.28847 0.41543 -0.02275
H*7 H 0.35466 0.42892 0.04532
H*8 H 0.30550 0.29438 -0.06781
N9 N -0.02437 0.70828 -0.16527
N10 N 0.25621 0.72911 0.10501
H*11 H 0.18060 0.75241 0.17173
H*12 H 0.00565 0.75652 -0.23854
H*13 H -0.14187 0.67394 -0.16602
H*14 H 0.32777 0.83479 0.09937
N'1+ N 0.48375 -0.00784 0.14123
N'2+ N 0.62060 0.17636 0.24634
N3+ N 0.48385 0.16224 0.18894
N'4+ N 0.62672 -0.11108 0.16817
C5+ C 0.70729 0.00224 0.23142
C6+ C 0.87027 -0.05478 0.27913
N'7+ N 0.95805 -0.22763 0.26500
N'8+ N 1.09687 -0.21890 0.32169
N'9+ N 1.09285 -0.04836 0.36792
N'10+ N 0.95116 0.05879 0.34258
O11+ O 0.36442 0.29800 0.18031

#END

S68. Optimized crystal structure coordinates for 5 polymorphs of **9g** (ionic form).

data_2TAGH_BTO_2_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 20.911
_cell_length_b 9.911

_cell_length_c 3.974
_cell_angle_alpha 86.78
_cell_angle_beta 80.63
_cell_angle_gamma 75.53
_cell_volume 786.737
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.58006 -0.29550 0.93173
N2 N 0.59721 -0.17369 0.92614
H*3 H 0.56026 -0.08493 0.92297
N4 N 0.62686 -0.41567 0.93607
H*5 H 0.67477 -0.40996 0.93493
N6 N 0.51611 -0.29714 0.93299
H*7 H 0.50516 -0.39161 0.93728
N8 N 0.60766 -0.54159 0.94188
N9 N 0.66439 -0.17479 0.92494
H*10 H 0.66899 -0.12572 1.13489
H*11 H 0.63177 -0.59781 0.73170
H*12 H 0.61890 -0.59770 1.15627
H*13 H 0.68186 -0.12582 0.71033
N14 N 0.46814 -0.17012 0.92837
H*15 H 0.44585 -0.16303 0.71631
H*16 H 0.43298 -0.16292 1.14088
C1 C 0.09995 0.19774 0.39015
N2 N 0.14239 0.07442 0.43447
H*3 H 0.18999 0.07459 0.45940
N4 N 0.03660 0.20337 0.35592
H*5 H 0.02271 0.11183 0.36501
N6 N 0.12086 0.31543 0.38006
H*7 H 0.08715 0.40680 0.34605
N8 N -0.00678 0.33356 0.30989
N9 N 0.11931 -0.04708 0.44409
H*10 H 0.12385 -0.09731 0.67289
H*11 H -0.02382 0.33689 0.08292
H*12 H -0.04613 0.35077 0.50361
H*13 H 0.14615 -0.11119 0.25220
N14 N 0.18731 0.30675 0.41647
H*15 H 0.21097 0.34670 0.20430
H*16 H 0.18867 0.36059 0.62499
N'1+ N 0.20810 0.50501 -0.13182
N'2+ N 0.17540 0.73538 -0.06081
N3+ N 0.15801 0.61345 -0.01958
N'4+ N 0.26104 0.55731 -0.25283
C5+ C 0.24036 0.69604 -0.20780
C6+ C 0.28283 0.79431 -0.30569
N'7+ N 0.34759 0.75669 -0.45225
N'8+ N 0.36689 0.87690 -0.49780
N'9+ N 0.31602 0.98223 -0.38373

```
N'10+ N 0.26213 0.93348 -0.26062
O11+ O 0.09919 0.60130 0.11420

#END

data_2TAGH_BTO_2_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                 20.788
_cell_length_b                 9.940
_cell_length_c                 4.004
_cell_angle_alpha               88.40
_cell_angle_beta                91.19
_cell_angle_gamma                75.22
_cell_volume                   799.337
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.89907 0.30036 0.02479
N2 N 0.87986 0.18146 0.03713
H*3 H 0.91540 0.09167 0.08955
N4 N 0.85417 0.42171 -0.04335
H*5 H 0.80608 0.41915 -0.08413
N6 N 0.96318 0.29791 0.08059
H*7 H 0.97572 0.39026 0.06896
N8 N 0.87552 0.54453 -0.05480
N9 N 0.81256 0.18682 -0.02212
H*10 H 0.79381 0.14868 0.18230
H*11 H 0.86561 0.59155 -0.28605
H*12 H 0.85187 0.61043 0.12013
H*13 H 0.80755 0.12979 -0.22388
N14 N 1.00913 0.16973 0.15129
H*15 H 1.04466 0.15141 -0.02497
H*16 H 1.03091 0.17030 0.38121
C1 C 0.58030 0.20471 0.00758
N2 N 0.62726 0.08493 0.05854
H*3 H 0.67512 0.09063 0.09053
N4 N 0.51639 0.20306 -0.03607
H*5 H 0.50560 0.10889 -0.02878
N6 N 0.59725 0.32613 0.00027
H*7 H 0.56018 0.41461 -0.03901
N8 N 0.46826 0.32967 -0.08890
N9 N 0.60826 -0.04059 0.06508
```

H*10 H 0.62089 -0.09093 0.29122
H*11 H 0.44467 0.33114 -0.31494
H*12 H 0.43442 0.34243 0.09546
H*13 H 0.63114 -0.10222 -0.11918
N14 N 0.66438 0.32505 0.04656
H*15 H 0.68046 0.36827 -0.15874
H*16 H 0.67022 0.37957 0.25165
N'1+ N 0.20997 0.00864 0.51052
N'2+ N 0.17734 0.23701 0.59347
N3+ N 0.16002 0.11602 0.59136
N'4+ N 0.26275 0.06069 0.45663
C5+ C 0.24210 0.19821 0.50778
C6+ C 0.28443 0.29582 0.47520
N'7+ N 0.34900 0.25873 0.39008
N'8+ N 0.36822 0.37801 0.38956
N'9+ N 0.31749 0.48231 0.47075
N'10+ N 0.26377 0.43378 0.52645
O11+ O 0.10139 0.10378 0.65992

#END

data_2TAGH_BTO_2_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 11.244
_cell_length_b 10.846
_cell_length_c 10.336
_cell_angle_alpha 136.04
_cell_angle_beta 84.73
_cell_angle_gamma 111.64
_cell_volume 783.323
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.19654 -0.00432 -0.30388
N2 N 0.07105 -0.14437 -0.38810
H*3 H 0.04178 -0.21678 -0.35414
N4 N 0.24021 0.09564 -0.34365
H*5 H 0.17512 0.06085 -0.43840
N6 N 0.27836 0.03577 -0.17989
H*7 H 0.37272 0.14297 -0.11910
N8 N 0.37180 0.24130 -0.25372
N9 N -0.01249 -0.18347 -0.51716

H*10 H -0.09227 -0.15804 -0.46778
H*11 H 0.42157 0.20627 -0.35548
H*12 H 0.37342 0.37482 -0.17296
H*13 H -0.04412 -0.32658 -0.65030
N14 N 0.23030 -0.07080 -0.14075
H*15 H 0.28439 -0.14547 -0.17964
H*16 H 0.23624 0.02308 0.00288
C1 C 0.16422 0.48581 0.20992
N2 N 0.20158 0.58578 0.17006
H*3 H 0.13125 0.55552 0.08458
N4 N 0.25308 0.52006 0.32197
H*5 H 0.34776 0.62295 0.37385
N6 N 0.03799 0.35159 0.13774
H*7 H 0.01365 0.27896 0.17133
N8 N 0.21153 0.41362 0.36148
N9 N 0.33410 0.72528 0.24726
H*10 H 0.33848 0.86146 0.33359
H*11 H 0.26361 0.33356 0.31142
H*12 H 0.22597 0.50819 0.50671
H*13 H 0.37613 0.68683 0.13830
N14 N -0.05297 0.31853 0.02102
H*15 H -0.09061 0.17509 -0.11289
H*16 H -0.12826 0.34972 0.08239
N'1+ N 0.41593 0.10355 0.39011
N'2+ N 0.34808 0.17535 0.26350
N3+ N 0.31431 0.10547 0.33461
N'4+ N 0.52177 0.17533 0.35424
C5+ C 0.47891 0.21766 0.27811
C6+ C 0.56330 0.30014 0.21744
N'7+ N 0.69371 0.34301 0.23110
N'8+ N 0.73134 0.41390 0.16074
N'9+ N 0.62818 0.41371 0.10709
N'10+ N 0.52040 0.34264 0.14106
O11+ O 0.19630 0.04605 0.34844

#END

data_2TAGH_BTO_2_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 12.422
_cell_length_b 11.240
_cell_length_c 10.342
_cell_angle_alpha 95.28
_cell_angle_beta 123.02
_cell_angle_gamma 125.75

```
_cell_volume                    783.802
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.48573 0.32157 0.70986
N2 N 0.58550 0.38410 0.66979
H*3 H 0.55559 0.42457 0.58476
N4 N 0.51954 0.26646 0.82134
H*5 H 0.62196 0.27424 0.87265
N6 N 0.35215 0.31415 0.63845
H*7 H 0.27964 0.26590 0.67217
N8 N 0.41332 0.20166 0.86109
N9 N 0.72434 0.39048 0.74619
H*10 H 0.86068 0.52231 0.83252
H*11 H 0.33283 0.06923 0.81067
H*12 H 0.50801 0.28170 1.00625
H*13 H 0.68549 0.30984 0.63695
N14 N 0.31953 0.37257 0.52230
H*15 H 0.17610 0.26693 0.38860
H*16 H 0.35128 0.47940 0.58417
C1 C -0.00441 0.79907 0.19627
N2 N 0.03518 0.75680 0.31968
H*3 H 0.14182 0.76907 0.37984
N4 N -0.14371 0.78526 0.11289
H*5 H -0.21595 0.74226 0.14702
N6 N 0.09530 0.85515 0.15625
H*7 H 0.06090 0.88589 0.06195
N8 N -0.18231 0.83026 -0.01558
N9 N -0.07110 0.69852 0.35910
H*10 H 0.02297 0.78639 0.50273
H*11 H -0.32547 0.71897 -0.14855
H*12 H -0.15617 0.93595 0.03439
H*13 H -0.14633 0.56942 0.31979
N14 N 0.24018 0.86843 0.24529
H*15 H 0.20462 0.78336 0.14316
H*16 H 0.37392 1.00033 0.32610
N'1+ N 0.10345 -0.31288 0.89011
N'2+ N 0.17421 -0.17376 0.76270
N3+ N 0.10435 -0.21007 0.83381
N'4+ N 0.17590 -0.34622 0.85481
C5+ C 0.21759 -0.26137 0.77818
C6+ C 0.30049 -0.26271 0.71786
N'7+ N 0.34443 -0.34933 0.73239
N'8+ N 0.41532 -0.31585 0.66206
N'9+ N 0.41412 -0.21361 0.60760
N'10+ N 0.34234 -0.17764 0.64099
O11+ O 0.04407 -0.15230 0.84692

#END
```

```
data_2TAGH_BTO_2_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                  20.246
_cell_length_b                  10.320
_cell_length_c                  4.007
_cell_angle_alpha                93.34
_cell_angle_beta                 80.07
_cell_angle_gamma                106.62
_cell_volume                    790.187
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.40133 0.78361 0.36632
N2 N -0.37441 0.68636 0.21578
H*3 H -0.32167 0.70973 0.14658
N4 N -0.47056 0.75810 0.46264
H*5 H -0.50085 0.66378 0.41701
N6 N -0.35902 0.90637 0.42054
H*7 H -0.38147 0.97732 0.53537
N8 N -0.49740 0.86146 0.61948
N9 N -0.41974 0.55890 0.16198
H*10 H -0.40811 0.48707 0.28644
H*11 H -0.53052 0.88234 0.47950
H*12 H -0.52339 0.83274 0.85638
H*13 H -0.41525 0.53667 -0.09044
N14 N -0.28684 0.93047 0.31750
H*15 H -0.26892 1.00622 0.14458
H*16 H -0.26178 0.95662 0.52146
C1 C 0.10953 0.28156 0.92752
N2 N 0.14435 0.18868 0.84241
H*3 H 0.19741 0.22138 0.80084
N4 N 0.03949 0.24383 0.98513
H*5 H 0.01474 0.14387 0.96167
N6 N 0.14475 0.41217 0.95502
H*7 H 0.11644 0.47943 1.02006
N8 N 0.00433 0.34285 1.07373
N9 N 0.10632 0.05283 0.81533
H*10 H 0.11828 -0.00388 0.98323
H*11 H -0.02633 0.34466 0.89852
H*12 H -0.02578 0.32281 1.30627
H*13 H 0.11773 0.01798 0.57549
```

N14 N 0.21794 0.44900 0.89350
H*15 H 0.23636 0.51482 0.69693
H*16 H 0.23691 0.49297 1.10468
N'1+ N 0.60705 0.19637 -0.20690
N'2+ N 0.70791 0.35404 -0.36449
N3+ N 0.63798 0.32270 -0.31683
N'4+ N 0.65875 0.14152 -0.18049
C5+ C 0.71901 0.23796 -0.27642
C6+ C 0.78894 0.22049 -0.28552
N'7+ N 0.80081 0.10552 -0.19857
N'8+ N 0.87078 0.13318 -0.24334
N'9+ N 0.89976 0.25921 -0.35240
N'10+ N 0.84941 0.31717 -0.38170
O11+ O 0.60378 0.40529 -0.37089

#END

S69. Optimized crystal structure coordinates for first energy polymorph of **1a** for cocrystal form.

data_NH3_BTO_0H_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 23.244
_cell_length_b 4.988
_cell_length_c 13.202
_cell_angle_alpha 90.00
_cell_angle_beta 118.94
_cell_angle_gamma 90.00
_cell_volume 1339.52
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.38416 0.81207 0.06834
H*2 H 0.40269 0.63676 0.05664
H*3 H 0.41545 0.96053 0.07292
H*4 H 0.34070 0.84480 -0.00506
N'1+ N -0.00905 0.67113 0.10794
N'2+ N 0.05275 1.02926 0.17384
N'3+ N -0.00916 0.93097 0.11034

N4+ N 0.05423 0.59508 0.17112
C5+ C 0.09170 0.81695 0.21112
C6+ C 0.16234 0.81827 0.28250
N'7+ N 0.20129 0.60596 0.31978
N'8+ N 0.26320 0.70425 0.38328
N'9+ N 0.26309 0.96409 0.38568
N10+ N 0.19981 1.04014 0.32250
H*11+ H 0.06782 0.39961 0.18296
H*12+ H 0.18622 1.23561 0.31066

#END

S70. Optimized crystal structure coordinates for first energy polymorph of **1b** for cocrystal form.

data_NH2OH_BTO_0H_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 7.923
_cell_length_b 20.270
_cell_length_c 5.001
_cell_angle_alpha 90.00
_cell_angle_beta 118.91
_cell_angle_gamma 90.00
_cell_volume 703.067
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.05885 -0.04239 0.20532
H*2 H 0.02255 -0.05440 0.43094
H*3 H 0.02309 -0.05466 0.10563
O4 O -0.05869 0.02893 0.20453
H*5 H -0.19445 0.03938 0.09999
N'1+ N -0.08526 0.57618 -0.55740
N'2+ N 0.06479 0.61416 -0.79599
N'3+ N -0.09105 0.58099 -0.82021
N4+ N 0.07772 0.60677 -0.35431
C5+ C 0.16860 0.62989 -0.50376
C6+ C 0.34874 0.66567 -0.36414
N'7+ N 0.45255 0.68140 -0.07191
N'8+ N 0.60839 0.71457 -0.04769
N'9+ N 0.60260 0.71938 -0.31050
N10+ N 0.43962 0.68879 -0.51359
H*11+ H 0.11651 0.60999 -0.12966

H*12+ H 0.40083 0.68557 -0.73824

#END

S71. Optimized crystal structure coordinates for first energy polymorph of **1c** for cocrystal form.

```
data_N2H4_BTO_0H_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/a'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a                 15.476
_cell_length_b                 7.250
_cell_length_c                 6.928
_cell_angle_alpha               90.00
_cell_angle_beta                69.51
_cell_angle_gamma                 90.00
_cell_volume                   728.15
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.20329 0.38701 0.25195
H*2 H 0.17295 0.26074 0.28944
H*3 H 0.20491 0.41893 0.10781
N4 N 0.29675 0.38695 0.24787
H*5 H 0.29514 0.41896 0.39198
H*6 H 0.32702 0.26060 0.21052
N'1+ N 0.36301 0.38580 0.59197
N'2+ N 0.43981 0.47449 0.78805
N'3+ N 0.37589 0.51997 0.70266
N4+ N 0.41950 0.24832 0.60400
C5+ C 0.46630 0.30453 0.72490
C6+ C 0.53368 0.19551 0.77508
N'7+ N 0.56017 0.02555 0.71193
N'8+ N 0.62409 -0.01993 0.79732
N'9+ N 0.63697 0.11424 0.90801
N10+ N 0.58048 0.25172 0.89598
H*11+ H 0.42267 0.12641 0.53021
H*12+ H 0.57731 0.37363 0.96977

#END
```

S72. Optimized crystal structure coordinates for first energy polymorph of **1d** for cocrystal form.

```
data_G_BTO_0H_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 13.156
_cell_length_b 9.893
_cell_length_c 7.502
_cell_angle_alpha 90.00
_cell_angle_beta 54.21
_cell_angle_gamma 90.00
_cell_volume 792.025
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74972 -0.51622 -0.49249
N'2 N 0.78098 -0.63385 -0.46723
H*3 H 0.81280 -0.62956 -0.37173
N4 N 0.71704 -0.49773 -0.63725
H*5 H 0.64399 -0.43420 -0.58328
H*6 H 0.70824 -0.58671 -0.69391
N7 N 0.74242 -0.39636 -0.38662
H*8 H 0.78104 -0.40183 -0.30330
H*9 H 0.76750 -0.31157 -0.47933
N'1+ N -0.12316 0.68084 -0.20692
N'2+ N -0.07536 0.85930 -0.09685
N'3+ N -0.12347 0.81186 -0.20312
N4+ N -0.07384 0.64032 -0.10104
C5+ C -0.04486 0.75091 -0.03423
C6+ C 0.01012 0.74915 0.08531
N'7+ N 0.04062 0.64076 0.14793
N'8+ N 0.08873 0.68820 0.25420
N'9+ N 0.08842 0.81922 0.25800
N10+ N 0.03910 0.85974 0.15212
H*11+ H -0.06309 0.54129 -0.08106
H*12+ H 0.02835 0.95877 0.13214

#END

S73. Optimized crystal structure coordinates for first energy polymorph of **1e** for cocrystal form.

data_AGXR_BTO_0H_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/c'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz

1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a 4.895
_cell_length_b 8.829
_cell_length_c 20.751
_cell_angle_alpha 90.00
_cell_angle_beta 94.46
_cell_angle_gamma 90.00
_cell_volume 894.1
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.54665 0.15484 0.57032
N2 N -0.56938 0.30916 0.55656
H*3 H -0.64308 0.33193 0.51052
N'4 N -0.32721 0.10461 0.60202
N5 N -0.76946 0.06823 0.54758
H*6 H -0.95187 0.12268 0.54689
H*7 H -0.76705 -0.03478 0.56963
N8 N -0.35226 -0.05429 0.61801
H*9 H -0.25629 -0.11412 0.58411
H*10 H -0.23204 -0.06869 0.65985
H*11 H -0.39130 0.36458 0.56874
N'1+ N 0.09718 -0.22945 0.09255
N'2+ N -0.09788 -0.00619 0.09368
N'3+ N -0.09327 -0.14430 0.06488
N4+ N 0.22174 -0.14629 0.14073
C5+ C 0.10000 -0.00936 0.14091
C6+ C 0.17592 0.11180 0.18553
N'7+ N 0.37380 0.10863 0.23276
N'8+ N 0.36919 0.24674 0.26156
N'9+ N 0.17874 0.33189 0.23389
N10+ N 0.05418 0.24873 0.18571
H*11+ H 0.37971 -0.18727 0.17010
H*12+ H -0.10379 0.28971 0.15634

#END

S74. Optimized crystal structure coordinates for first energy polymorph of **1f** for cocrystal form.

data_DAGXR_BTO_0H_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 19.033
_cell_length_b 7.705
_cell_length_c 6.661
_cell_angle_alpha 90.00
_cell_angle_beta 109.53
_cell_angle_gamma 90.00
_cell_volume 920.63
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.10376 0.68098 0.73738
N'2 N 0.03427 0.72522 0.67148
N3 N 0.13548 0.60787 0.59568
H*4 H 0.17093 0.50902 0.66096
N5 N 0.15244 0.69588 0.94493
N6 N 0.08824 0.56359 0.38767
N7 N 0.01329 0.80946 0.83643
H*8 H -0.00156 0.71501 0.92260
H*9 H 0.03670 0.53331 0.39438
H*10 H 0.08079 0.67348 0.29793
H*11 H -0.03475 0.87405 0.75889
H*12 H 0.20621 0.71706 0.95620
H*13 H 0.13311 0.78279 1.02906
N'1+ N 0.08140 0.29725 0.90225
N'2+ N 0.19123 0.18557 0.94342
N'3+ N 0.14890 0.27908 1.03309
N4+ N 0.07880 0.21413 0.72192
C5+ C 0.14661 0.14609 0.74927
C6+ C 0.16611 0.04721 0.59127
N'7+ N 0.12149 0.00773 0.39712
N'8+ N 0.16382 -0.08578 0.30745
N'9+ N 0.23132 -0.10395 0.43829
N10+ N 0.23392 -0.02083 0.61862
H*11+ H 0.03168 0.20891 0.59317
H*12+ H 0.28104 -0.01561 0.74737

#END

S75. Optimized crystal structure coordinates for first energy polymorph of **1g** for cocrystal form.

data_TAGXR_BTO_0H_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 9.113
_cell_length_b 30.066
_cell_length_c 5.386
_cell_angle_alpha 90.00
_cell_angle_beta 46.34
_cell_angle_gamma 90.00
_cell_volume 1067.61
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.14929 0.07595 0.43653
N'2 N 0.14913 0.10491 0.61527
N3 N -0.02910 0.13279 0.81556
N4 N -0.01220 0.07069 0.46073
N5 N 0.02535 0.04579 0.19818
N6 N 0.31373 0.04807 0.21228
N7 N 0.45675 0.04340 0.23882
H*8 H 0.00217 0.15867 0.89438
H*9 H -0.14644 0.11598 1.03471
H*10 H -0.08980 0.09986 0.53303
H*11 H -0.10561 0.03046 0.30086
H*12 H 0.07251 0.06581 0.00150
H*13 H 0.28598 0.01979 0.14906
H*14 H 0.54777 0.07080 0.12733
H*15 H 0.38146 0.04562 0.49266
N'1+ N -0.09595 0.61020 0.47748
N'2+ N -0.03859 0.66167 0.13108
N'3+ N -0.16141 0.62796 0.34973
N4+ N 0.07383 0.63256 0.34102
C5+ C 0.10742 0.66409 0.12867
C6+ C 0.27534 0.69495 -0.06617
N'7+ N 0.42135 0.69737 -0.06858
N'8+ N 0.54417 0.73108 -0.28723
N'9+ N 0.47871 0.74884 -0.41498
N10+ N 0.30893 0.72648 -0.27852
H*11+ H 0.15523 0.62508 0.40001
H*12+ H 0.22753 0.73396 -0.33751

#END

S76. Optimized crystal structure coordinates for first energy polymorph of **2a** for cocrystal form.

data_NH3_BTO_1H_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz

```
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a                 15.688
_cell_length_b                 8.813
_cell_length_c                 5.777
_cell_angle_alpha               90.00
_cell_angle_beta               121.39
_cell_angle_gamma                90.00
_cell_volume                   681.819
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.19772 0.03287 0.47603
H*2 H -0.25118 -0.01183 0.29501
H*3 H -0.23317 0.10391 0.53821
H*4 H -0.16969 -0.05448 0.61128
N'1+ N -0.16153 0.22038 -0.02993
N2+ N -0.13216 0.37874 0.27513
N'3+ N -0.18878 0.35388 0.01072
N'4+ N -0.08839 0.15917 0.20393
C5+ C -0.07011 0.25963 0.39601
C6+ C 0.00023 0.25498 0.68348
N7+ N 0.06586 0.14508 0.82985
N'8+ N 0.11710 0.18848 1.09328
N'9+ N 0.08296 0.32013 1.10309
N'10+ N 0.00998 0.36550 0.85163
O11+ O -0.14138 0.50883 0.38689
H*12+ H -0.09143 0.49870 0.58315
H*13+ H 0.07907 0.04460 0.76888

#END
```

S77. Optimized crystal structure coordinates for first energy polymorph of **2b** for cocrystal form.

```
data_NH2OH_BTO_1H_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                 6.403
_cell_length_b                 10.757
_cell_length_c                 5.511
_cell_angle_alpha               94.67
_cell_angle_beta               111.11
_cell_angle_gamma                96.32
```

_cell_volume 348.943
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.04753 -0.38123 0.71805
H*2 H -0.06442 -0.32651 0.74678
H*3 H 0.02117 -0.38516 0.52311
O4 O -0.04145 -0.50686 0.74356
H*5 H 0.08562 -0.53193 0.87820
N'1+ N -0.72066 0.26555 1.08357
N2+ N -0.56215 0.33267 0.83547
N'3+ N -0.69859 0.36149 0.95714
N'4+ N -0.60068 0.17565 1.04508
C5+ C -0.50087 0.21850 0.88824
C6+ C -0.35280 0.16263 0.78228
N7+ N -0.27831 0.05095 0.81767
N'8+ N -0.14222 0.03665 0.68098
N'9+ N -0.13606 0.13678 0.56786
N'10+ N -0.26523 0.21761 0.62623
O11+ O -0.50347 0.41304 0.68470
H*12+ H -0.40244 0.36952 0.61814
H*13+ H -0.31057 -0.01574 0.92444

#END

S78. Optimized crystal structure coordinates for first energy polymorph of **2c** for cocrystal form.

data_N2H4_BTO_1H_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 11.961
_cell_length_b 11.001
_cell_length_c 12.496
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1644.26
loop_
_atom_site_label

_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.45182 0.60796 -0.15167
H*2 H 0.43101 0.52012 -0.16866
H*3 H 0.53398 0.60953 -0.13085
N4 N 0.38897 0.65513 -0.06293
H*5 H 0.31779 0.69265 -0.09272
H*6 H 0.36637 0.58848 -0.01046
N'1+ N -0.15829 0.22404 0.60713
N2+ N -0.00409 0.29116 0.66213
N'3+ N -0.11221 0.31679 0.65657
N'4+ N -0.08157 0.13934 0.58089
C5+ C 0.01569 0.18217 0.61580
C6+ C 0.12605 0.13069 0.60998
N7+ N 0.15780 0.02429 0.56673
N'8+ N 0.26975 0.01266 0.57925
N'9+ N 0.30347 0.10919 0.62843
N'10+ N 0.21633 0.18501 0.64899
O11+ O 0.06879 0.36950 0.70928
H*12+ H 0.14254 0.32917 0.70270
H*13+ H 0.11134 -0.04044 0.52995

#END

S79. Optimized crystal structure coordinates for first energy polymorph of **2d** for cocrystal form.

data_G_BTO_1H_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 7.396
_cell_length_b 10.309
_cell_length_c 14.185
_cell_angle_alpha 90.00
_cell_angle_beta 53.41
_cell_angle_gamma 90.00
_cell_volume 868.392
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.25694 0.76353 0.92922
N'2 N 0.21038 0.73484 0.85774

H*3 H 0.17121 0.81568 0.83178
N4 N 0.29043 0.66566 0.98517
H*5 H 0.41730 0.68210 0.99204
H*6 H 0.29809 0.57671 0.95258
N7 N 0.28220 0.88751 0.96005
H*8 H 0.23028 0.96046 0.93373
H*9 H 0.22717 0.89724 1.04444
N'1+ N -0.41959 0.68429 0.05665
N2+ N -0.29536 0.78758 0.13477
N'3+ N -0.38280 0.80230 0.07665
N'4+ N -0.35724 0.59410 0.10096
C5+ C -0.27888 0.65984 0.15021
C6+ C -0.18951 0.61445 0.21071
N7+ N -0.16338 0.49159 0.23234
N'8+ N -0.07291 0.49421 0.29183
N'9+ N -0.04612 0.61491 0.30514
N'10+ N -0.11685 0.69292 0.25575
O11+ O -0.23687 0.89227 0.16954
H*12+ H -0.17711 0.85483 0.21024
H*13+ H -0.20060 0.40711 0.21085

#END

S80. Optimized crystal structure coordinates for first energy polymorph of **2e** for cocrystal form.

data_AGXR_BTO_1H_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 17.610
_cell_length_b 7.480
_cell_length_c 9.641
_cell_angle_alpha 83.53
_cell_angle_beta 49.70
_cell_angle_gamma 126.14
_cell_volume 466.92
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.42091 0.19224 -0.21811
N2 N 0.60442 0.38583 -0.44660
H*3 H 0.71325 0.61539 -0.53447
N'4 N 0.33132 0.07442 -0.22028
N5 N 0.35160 0.14572 -0.00539
H*6 H 0.38638 0.12034 0.03731
H*7 H 0.20113 -0.05597 0.18472

N8 N 0.13268 -0.15437 0.05077
H*9 H 0.15283 0.01163 -0.00677
H*10 H 0.04676 -0.33573 0.08722
H*11 H 0.65800 0.44260 -0.61129
N'1+ N -0.03488 0.05656 0.23525
N2+ N 0.05623 0.25738 0.31459
N'3+ N -0.09850 0.02960 0.42899
N'4+ N 0.15804 0.29777 -0.00152
C5+ C 0.21489 0.42385 0.04966
C6+ C 0.40446 0.68663 -0.12634
N7+ N 0.57346 0.87181 -0.39121
N'8+ N 0.71505 1.08983 -0.47482
N'9+ N 0.63269 1.03581 -0.26602
N'10+ N 0.43903 0.78621 -0.04475
O11+ O 0.04103 0.29650 0.46112
H*12+ H 0.17514 0.47922 0.32962
H*13+ H 0.60164 0.86457 -0.51924

#END

S81. Optimized crystal structure coordinates for first energy polymorph of **2f** for cocrystal form.

data_DAGXR_BTO_1H_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 10.086
_cell_length_b 14.991
_cell_length_c 6.857
_cell_angle_alpha 90.00
_cell_angle_beta 77.12
_cell_angle_gamma 90.00
_cell_volume 1010.69
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.02670 0.56802 0.76040
N'2 N 0.00348 0.65084 0.80831
N3 N 0.16036 0.53745 0.69766
H*4 H 0.17209 0.49372 0.58225
N5 N -0.07162 0.50319 0.76086
N6 N 0.26779 0.60059 0.66383
N7 N -0.13960 0.66808 0.88272
H*8 H -0.18104 0.68133 0.76248

H*9 H 0.23177 0.65954 0.62075
H*10 H 0.29028 0.61317 0.79884
H*11 H -0.14424 0.72675 0.95844
H*12 H -0.04292 0.44090 0.79179
H*13 H -0.16276 0.52199 0.84785
N'1+ N -0.21371 0.17039 0.44436
N2+ N -0.13295 0.23202 0.66774
N'3+ N -0.21474 0.24542 0.54373
N'4+ N -0.13264 0.10908 0.50252
C5+ C -0.08187 0.14834 0.64363
C6+ C 0.01038 0.11494 0.75884
N7+ N 0.06863 0.03400 0.75090
N'8+ N 0.14816 0.03173 0.88598
N'9+ N 0.13748 0.10895 0.97155
N'10+ N 0.05246 0.16272 0.89635
O11+ O -0.11092 0.29745 0.79421
H*12+ H -0.04721 0.27052 0.86855
H*13+ H 0.05971 -0.01924 0.66363

#END

S82. Optimized crystal structure coordinates for first energy polymorph of **2g** for cocrystal form.

data_TAGXR_BTO_1H_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 21.712
_cell_length_b 7.526
_cell_length_c 6.835
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1116.87
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.64713 0.24857 0.30126
N'2 N 0.58795 0.22666 0.29089
N3 N 0.56669 0.22659 0.09069
N4 N 0.68508 0.25623 0.13696
N5 N 0.74565 0.32165 0.16483
N6 N 0.67552 0.26324 0.48139
N7 N 0.64335 0.21126 0.65171

H*8 H 0.52021 0.24089 0.09949
H*9 H 0.57372 0.10248 0.03333
H*10 H 0.66105 0.30273 0.01931
H*11 H 0.77375 0.26129 0.06635
H*12 H 0.74756 0.45578 0.14438
H*13 H 0.72103 0.23499 0.48351
H*14 H 0.61358 0.31155 0.68501
H*15 H 0.61576 0.10545 0.61705
N'1+ N -0.11134 0.15399 -0.04198
N2+ N -0.15426 0.26659 -0.28827
N'3+ N -0.16556 0.19347 -0.11554
N'4+ N -0.06545 0.20056 -0.16460
C5+ C -0.09280 0.27162 -0.31995
C6+ C -0.06685 0.34422 -0.49626
N7+ N -0.00723 0.35778 -0.54706
N'8+ N -0.00402 0.43469 -0.72590
N'9+ N -0.06001 0.46586 -0.77969
N'10+ N -0.10053 0.41135 -0.64044
O11+ O -0.20108 0.32353 -0.40462
H*12+ H -0.18036 0.37159 -0.52247
H*13+ H 0.03104 0.32029 -0.47289

#END

S83. Optimized crystal structure coordinates for first energy polymorph of **3a** for cocrystal form.

data_00173_-4.32294E+01
_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 7.133
_cell_length_b 22.309
_cell_length_c 4.864
_cell_angle_alpha 90.00
_cell_angle_beta 64.68
_cell_angle_gamma 90.00
_cell_volume 699.652
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.21498 0.54642 0.15411
H*2 H -0.30106 0.57609 0.31925
H*3 H -0.10642 0.57075 -0.01757
H*4 H -0.13713 0.52034 0.24289

N'1+ N 0.20412 0.04260 0.71888
N'2+ N 0.24113 0.13125 0.90390
N3+ N 0.14199 0.08028 0.95074
N'4+ N 0.35812 0.07033 0.49650
C5+ C 0.37873 0.12381 0.61151
C6+ C 0.52945 0.16984 0.44881
N'7+ N 0.67282 0.16898 0.16420
N'8+ N 0.77369 0.22229 0.12074
N'9+ N 0.69835 0.25504 0.36424
N10+ N 0.54378 0.22270 0.57434
O11+ O -0.01600 0.06795 1.22575
H*12+ H 0.45911 0.23854 0.78699
H*13+ H -0.06220 0.02807 1.20067

#END

S84. Optimized crystal structure coordinates for first energy polymorph of **3b** for cocrystal form.

data_09339_-5.36852E+01
_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 11.048
_cell_length_b 6.431
_cell_length_c 5.513
_cell_angle_alpha 84.96
_cell_angle_beta 103.23
_cell_angle_gamma 103.46
_cell_volume 370.58
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.05449 -0.38244 0.26557
H*2 H 0.02654 -0.26088 0.15042
H*3 H -0.02752 -0.49246 0.27682
O4 O 0.09585 -0.29119 0.50919
H*5 H 0.18159 -0.31323 0.56230
N'1+ N 0.17642 0.17974 0.54473
N'2+ N 0.22009 0.18576 0.16757
N3+ N 0.13415 0.16809 0.30069
N'4+ N 0.30134 0.20762 0.57991
C5+ C 0.32636 0.21094 0.35050
C6+ C 0.45177 0.23807 0.29607
N'7+ N 0.56363 0.26425 0.45426
N'8+ N 0.65132 0.28222 0.31202
N'9+ N 0.59792 0.26820 0.07697

N10+ N 0.47178 0.24025 0.06287
O11+ O 0.00867 0.13935 0.18883
H*12+ H 0.40827 0.22466 -0.10263
H*13+ H -0.03406 0.13124 0.32671

#END

S85. Optimized crystal structure coordinates for first energy polymorph of **3c** for cocrystal form.

data_03907_-4.59589E+01
_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 17.748
_cell_length_b 10.222
_cell_length_c 6.388
_cell_angle_alpha 90.00
_cell_angle_beta 139.69
_cell_angle_gamma 90.00
_cell_volume 749.726
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.54931 0.94965 0.36648
H*2 H 0.53138 0.89691 0.19682
H*3 H 0.48165 1.01193 0.24793
N4 N 0.65284 1.02727 0.56304
H*5 H 0.72144 0.97163 0.75533
H*6 H 0.66704 1.05375 0.44129
N'1+ N 0.06421 0.71426 0.00868
N'2+ N 0.06613 0.87474 -0.22478
N3+ N 0.02258 0.82800 -0.14352
N'4+ N 0.14245 0.68117 0.03255
C5+ C 0.14268 0.77901 -0.10947
C6+ C 0.21536 0.78544 -0.14122
N'7+ N 0.29369 0.69984 -0.04119
N'8+ N 0.33770 0.75037 -0.12807
N'9+ N 0.28989 0.86171 -0.27488
N10+ N 0.21229 0.88565 -0.28569
O11+ O -0.06100 0.89504 -0.21501
H*12+ H 0.16288 0.96768 -0.38947
H*13+ H -0.07797 0.84013 -0.13010

#END

S86. Optimized crystal structure coordinates for first energy polymorph of **3d** for cocrystal form.

```
data_02034_-6.21611E+01
_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                  4.606
_cell_length_c                  18.235
_cell_angle_alpha                90.00
_cell_angle_beta                 80.78
_cell_angle_gamma                90.00
_cell_volume                    853.51
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.19154 0.09792 -0.11703
N'2 N 0.12975 -0.14520 -0.11400
H*3 H 0.13776 -0.25562 -0.06641
N4 N 0.20508 0.26689 -0.18124
H*5 H 0.19487 0.48358 -0.17242
H*6 H 0.14988 0.19067 -0.21832
N7 N 0.25010 0.22642 -0.06095
H*8 H 0.25760 0.09411 -0.01754
H*9 H 0.33410 0.33804 -0.07880
N'1+ N 0.12203 -0.12006 0.58120
N'2+ N 0.22258 -0.18436 0.67988
N3+ N 0.13290 -0.04729 0.65008
N'4+ N 0.21177 -0.32328 0.56279
C5+ C 0.27174 -0.35987 0.62292
C6+ C 0.37777 -0.56233 0.62866
N'7+ N 0.43562 -0.74649 0.57799
N'8+ N 0.52826 -0.88624 0.61012
N'9+ N 0.52898 -0.79556 0.67738
N10+ N 0.43456 -0.59073 0.69018
O11+ O 0.05635 0.15816 0.68922
H*12+ H 0.41515 -0.48486 0.73938
H*13+ H -0.00098 0.22508 0.65506

#END
```

S87. Optimized crystal structure coordinates for first energy polymorph of **3e** for cocrystal form.

```
data_02891_-6.13024E+01
_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                   10.403
_cell_length_b                   8.411
_cell_length_c                   8.656
_cell_angle_alpha                126.29
_cell_angle_beta                 130.64
_cell_angle_gamma                74.58
_cell_volume                     454.304
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.44298 0.16847 -0.05221
N2 N -0.28493 0.11321 0.06938
H*3 H -0.27399 -0.02070 -0.04628
N'4 N -0.52254 0.23990 0.03774
N5 N -0.50059 0.13937 -0.26495
H*6 H -0.40522 0.15792 -0.25977
H*7 H -0.59540 0.21781 -0.31635
N8 N -0.67387 0.30939 -0.09626
H*9 H -0.77801 0.19703 -0.22086
H*10 H -0.68850 0.42278 0.03038
H*11 H -0.25707 0.11940 0.20927
N'1+ N -0.18975 0.18162 0.52322
N'2+ N -0.22439 0.34065 0.80804
N3+ N -0.28283 0.28517 0.59269
N'4+ N -0.05728 0.16560 0.70667
C5+ C -0.07990 0.26234 0.87739
C6+ C 0.03444 0.28419 1.11241
N'7+ N 0.17940 0.21629 1.20489
N'8+ N 0.23768 0.27561 1.42824
N'9+ N 0.13532 0.37546 1.47449
N10+ N 0.00601 0.38259 1.27711
O11+ O -0.43180 0.33362 0.45179
H*12+ H -0.09202 0.45313 1.26749
H*13+ H -0.44596 0.27573 0.30408

#END
```

S88. Optimized crystal structure coordinates for first energy polymorph of **3f** for cocrystal form.

```
data_06721_-5.93665E+01
_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                 13.409
_cell_length_b                 7.703
_cell_length_c                 10.251
_cell_angle_alpha               90.00
_cell_angle_beta                78.98
_cell_angle_gamma                 90.00
_cell_volume                   1039.3
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.26098 0.76094 0.53856
N'2 N 0.16295 0.75331 0.55891
N3 N 0.31614 0.63031 0.58757
H*4 H 0.37547 0.67700 0.62519
N5 N 0.32039 0.89306 0.47213
N6 N 0.26252 0.50278 0.67324
N7 N 0.12034 0.89238 0.49279
H*8 H 0.11093 0.99735 0.55515
H*9 H 0.19692 0.55738 0.72424
H*10 H 0.23995 0.40997 0.61430
H*11 H 0.04878 0.85292 0.48778
H*12 H 0.38981 0.85372 0.42368
H*13 H 0.28129 0.96187 0.41363
N'1+ N 0.07210 0.32133 0.45524
N'2+ N 0.17148 0.36061 0.25610
N3+ N 0.07962 0.35417 0.32715
N'4+ N 0.16670 0.30410 0.47241
C5+ C 0.22589 0.32815 0.35131
C6+ C 0.33614 0.32129 0.32128
N'7+ N 0.39927 0.29112 0.40340
N'8+ N 0.49409 0.29844 0.32752
N'9+ N 0.49110 0.33141 0.20429
N10+ N 0.39194 0.34632 0.19823
O11+ O -0.00237 0.38038 0.26958
H*12+ H 0.36898 0.37225 0.11174
H*13+ H -0.06025 0.36883 0.34268

#END
```

S89. Optimized crystal structure coordinates for first energy polymorph of **3g** for cocrystal form.

```
data_01363_-6.15928E+01
_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 9.066
_cell_length_b 11.765
_cell_length_c 11.168
_cell_angle_alpha 90.00
_cell_angle_beta 118.25
_cell_angle_gamma 90.00
_cell_volume 1049.31
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.31679 -0.44381 0.87524
N'2 N 0.27616 -0.40363 0.96383
N3 N 0.17815 -0.48409 0.99416
N4 N 0.28050 -0.55458 0.82541
N5 N 0.29554 -0.57930 0.70746
N6 N 0.40203 -0.37644 0.82710
N7 N 0.48031 -0.27573 0.89735
H*8 H 0.12846 -0.43839 1.04368
H*9 H 0.25820 -0.54102 1.06415
H*10 H 0.17636 -0.58364 0.82858
H*11 H 0.32901 -0.66216 0.71159
H*12 H 0.18517 -0.56610 0.62127
H*13 H 0.46597 -0.41855 0.78737
H*14 H 0.38869 -0.21604 0.87142
H*15 H 0.52377 -0.28930 0.99914
N'1+ N -0.08521 0.30226 0.88131
N'2+ N 0.00078 0.12287 0.93774
N3+ N -0.09391 0.20612 0.93892
N'4+ N 0.02445 0.28253 0.83746
C5+ C 0.07533 0.17385 0.87224
C6+ C 0.19640 0.11430 0.84475
N'7+ N 0.27909 0.15274 0.78214
N'8+ N 0.37648 0.06496 0.78211
N'9+ N 0.35652 -0.02405 0.84140
N10+ N 0.24317 0.00536 0.88173
O11+ O -0.19469 0.19204 0.99707
H*12+ H 0.20549 -0.04999 0.93123
H*13+ H -0.25054 0.26519 0.98445

#END

S90. Optimized crystal structure coordinates for first energy polymorph of **4a** for cocrystal form.
data_01239_-3.60994E+01

```
_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                 18.612
_cell_length_b                 8.703
_cell_length_c                 4.618
_cell_angle_alpha               90.00
_cell_angle_beta                69.24
_cell_angle_gamma                 90.00
_cell_volume                   699.458
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.35064 0.12465 -0.32266
H*2 H 0.30938 0.06807 -0.37846
H*3 H 0.37832 0.19529 -0.50397
H*4 H 0.32286 0.19348 -0.13835
N'1+ N -0.05178 0.13545 0.91513
N2+ N 0.01881 0.29638 1.02739
N'3+ N -0.05175 0.23687 1.12437
N'4+ N 0.01757 0.12853 0.68480
C5+ C 0.06149 0.23042 0.75831
C6+ C 0.14013 0.26636 0.58747
N7+ N 0.18281 0.20040 0.31839
N'8+ N 0.25337 0.25991 0.22141
N'9+ N 0.25340 0.36133 0.43065
N'10+ N 0.18405 0.36825 0.66098
O11+ O 0.03874 0.40694 1.19349
O12+ O 0.16288 0.08984 0.15229
H*13+ H 0.09295 0.43074 1.07374
H*14+ H 0.10867 0.06604 0.27204

#END
```

S91. Optimized crystal structure coordinates for first energy polymorph of **4b** for cocrystal form.

```
data_04172_-4.46839E+01
_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 23.369
_cell_length_b 7.146
_cell_length_c 10.262
_cell_angle_alpha 90.00
_cell_angle_beta 71.26
_cell_angle_gamma 90.00
_cell_volume 1622.85
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N'1 N -0.08209 0.08981 -0.40615
N2 N -0.14032 -0.06058 -0.48772
N'3 N -0.10719 0.09467 -0.50324
N'4 N -0.09848 -0.06595 -0.32827
C5 C -0.13515 -0.15943 -0.38071
C6 C -0.16457 -0.33395 -0.33431
N7 N -0.15940 -0.43280 -0.22730
N'8 N -0.19253 -0.58805 -0.21178
N'9 N -0.21763 -0.58319 -0.30887
N'10 N -0.20124 -0.42743 -0.38675
O11 O -0.17287 -0.09988 -0.57310
O12 O -0.12685 -0.39350 -0.14192
H*13 H -0.19291 -0.22023 -0.54019
H*14 H -0.10681 -0.27315 -0.17483
N1+ N -0.03632 0.39205 -0.08548
H*2+ H -0.05042 0.43937 -0.16411
H*3+ H -0.05021 0.49049 -0.00955
O4+ O 0.02856 0.41482 -0.13699
H*5+ H 0.04298 0.29058 -0.12772

#END

S92. Optimized crystal structure coordinates for first energy polymorph of **4c** for cocrystal form.

data_01361_-3.92482E+01
_symmetry_cell_setting orthorhombic
_symmetry_space_group_name_H-M 'P c a 21'
_symmetry_Int_Tables_number 29
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,y,1/2+z
3 1/2+x,-y,z

4 -x,-y,1/2+z
_cell_length_a 11.428
_cell_length_b 5.129
_cell_length_c 12.923
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 757.471
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.38803 0.15818 0.55802
H*2 H -0.46815 0.14397 0.52369
H*3 H -0.36775 -0.01967 0.58780
N4 N -0.38805 0.34179 0.64198
H*5 H -0.36778 0.51965 0.61221
H*6 H -0.46818 0.35595 0.67630
N'1+ N 0.03617 0.80478 0.24111
N2+ N 0.20132 0.98568 0.25085
N'3+ N 0.09800 0.99720 0.20322
N'4+ N 0.09785 0.66933 0.31238
C5+ C 0.20168 0.78525 0.31777
C6+ C 0.29832 0.71473 0.38223
N7+ N 0.29868 0.51430 0.44915
N'8+ N 0.40200 0.50278 0.49678
N'9+ N 0.46383 0.69520 0.45889
N'10+ N 0.40215 0.83065 0.38762
O11+ O 0.28764 1.16035 0.22926
O12+ O 0.21236 0.33963 0.47074
H*13+ H 0.35366 1.10990 0.27405
H*14+ H 0.14634 0.39008 0.42595

#END

S93. Optimized crystal structure coordinates for first energy polymorph of **4d** for cocrystal form.

data_____-5.16436E+01
_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 12.755
_cell_length_b 7.207
_cell_length_c 4.954
_cell_angle_alpha 90.00
_cell_angle_beta 106.81
_cell_angle_gamma 90.00

_cell_volume 435.938
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.24581 0.57583 0.06039
N'2 N 0.29577 0.54693 0.32190
H*3 H 0.37629 0.58387 0.36968
N4 N 0.13827 0.51551 -0.05490
H*5 H 0.08906 0.60477 -0.19300
H*6 H 0.10475 0.46945 0.09481
N7 N 0.28670 0.66675 -0.13740
H*8 H 0.36834 0.69043 -0.07216
H*9 H 0.26077 0.61516 -0.33604
N'1+ N 0.03849 -0.00888 0.78662
N2+ N 0.14044 0.15814 0.62029
N'3+ N 0.03829 0.09542 0.57022
N'4+ N 0.13903 -0.01450 0.97546
C5+ C 0.20246 0.09124 0.86818
C6+ C 0.31638 0.12990 0.98888
N7+ N 0.37840 0.06300 1.23677
N'8+ N 0.48055 0.12572 1.28684
N'9+ N 0.48035 0.23002 1.07044
N'10+ N 0.37981 0.23564 0.88160
O11+ O 0.16907 0.27228 0.43433
O12+ O 0.34977 -0.05114 1.42273
H*13+ H 0.24760 0.29793 0.51959
H*14+ H 0.27124 -0.07679 1.33747

#END

S94. Optimized crystal structure coordinates for first energy polymorph of **4e** for cocrystal form.
data_02067_-5.20595E+01
_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 12.179
_cell_length_b 10.642
_cell_length_c 7.201
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 933.314
loop_

_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.01885 -0.14042 -0.67456
N2 N -0.12363 -0.13866 -0.75274
H*3 H -0.18031 -0.09339 -0.67406
N'4 N 0.03704 -0.24378 -0.67631
N5 N 0.01551 -0.02715 -0.59993
H*6 H -0.01358 0.04973 -0.66679
H*7 H 0.09823 -0.02665 -0.57976
N8 N 0.14775 -0.22460 -0.60824
H*9 H 0.14834 -0.25181 -0.47201
H*10 H 0.19434 -0.28993 -0.67507
H*11 H -0.14870 -0.22619 -0.78899
N'1+ N -0.25610 0.33388 0.55867
N2+ N -0.16070 0.49482 0.50389
N'3+ N -0.26123 0.44668 0.48677
N'4+ N -0.15397 0.30844 0.62190
C5+ C -0.09470 0.41054 0.58656
C6+ C 0.01889 0.43039 0.62720
N7+ N 0.08489 0.34611 0.70986
N'8+ N 0.18541 0.39425 0.72699
N'9+ N 0.18029 0.50705 0.65508
N'10+ N 0.07816 0.53249 0.59186
O11+ O -0.13707 0.61270 0.44224
O12+ O 0.06126 0.22823 0.77152
H*13+ H -0.05872 0.62530 0.47094
H*14+ H -0.01709 0.21563 0.74281

#END

S95. Optimized crystal structure coordinates for first energy polymorph of **4f** for cocrystal form.

data_03331_-5.05236E+01
_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 7.698
_cell_length_b 18.692
_cell_length_c 7.049
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 1014.29
loop_

_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.15535 0.69590 -0.10986
N'2 N 0.20452 0.67110 -0.27233
N3 N 0.18785 0.65699 0.05573
H*4 H 0.08707 0.65820 0.14831
N5 N 0.06637 0.75955 -0.08070
N6 N 0.25513 0.58661 0.03953
N7 N 0.17087 0.72103 -0.42403
H*8 H 0.04658 0.71261 -0.47052
H*9 H 0.21268 0.56518 -0.08582
H*10 H 0.38639 0.59120 0.02581
H*11 H 0.24852 0.70508 -0.53286
H*12 H 0.09260 0.78340 0.04528
H*13 H 0.08009 0.79297 -0.19370
N'1+ N 0.63434 0.14792 -0.23386
N2+ N 0.87077 0.13423 -0.08775
N'3+ N 0.80065 0.16194 -0.24423
N'4+ N 0.59599 0.11164 -0.07334
C5+ C 0.74600 0.10336 0.01738
C6+ C 0.77431 0.06827 0.19492
N7+ N 0.64954 0.03740 0.30006
N'8+ N 0.71966 0.00969 0.45653
N'9+ N 0.88597 0.02370 0.44617
N'10+ N 0.92432 0.05999 0.28565
O11+ O 1.04433 0.13937 -0.05319
O12+ O 0.47598 0.03226 0.26549
H*13+ H 1.06226 0.11504 0.06929
H*14+ H 0.45806 0.05659 0.14301

#END

S96. Optimized crystal structure coordinates for first energy polymorph of **4g** for cocrystal form.

data_07397_-5.13564E+01
_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 6.161
_cell_length_b 12.156
_cell_length_c 15.264
_cell_angle_alpha 90.00
_cell_angle_beta 104.65
_cell_angle_gamma 90.00

```
_cell_volume                1106
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.09153 0.22470 0.74367
N'2 N -0.28702 0.27137 0.72002
N3 N -0.27209 0.38233 0.68826
N4 N 0.10365 0.27407 0.73225
N5 N 0.31040 0.22682 0.77954
N6 N -0.07008 0.12058 0.78111
N7 N -0.26331 0.05493 0.77314
H*8 H -0.42257 0.41735 0.68720
H*9 H -0.26517 0.37887 0.62197
H*10 H 0.08992 0.35765 0.73374
H*11 H 0.42383 0.23915 0.74246
H*12 H 0.36855 0.26201 0.84173
H*13 H 0.06816 0.07835 0.77677
H*14 H -0.34189 0.08268 0.82017
H*15 H -0.37280 0.07148 0.71196
N'1+ N -0.30652 0.82912 -0.00566
N2+ N 0.03713 0.82837 -0.00281
N'3+ N -0.14893 0.88899 -0.02551
N'4+ N -0.22526 0.73091 0.02945
C5+ C -0.00869 0.73149 0.03088
C6+ C 0.15149 0.64597 0.06212
N7+ N 0.10567 0.54909 0.09581
N'8+ N 0.29173 0.48847 0.11851
N'9+ N 0.44932 0.54834 0.09866
N'10+ N 0.36806 0.64655 0.06355
O11+ O 0.23534 0.86663 -0.01475
O12+ O -0.09254 0.51083 0.10775
H*13+ H 0.34425 0.80711 0.00698
H*14+ H -0.20145 0.57035 0.08602

#END
```

S97. Optimized crystal structure coordinates for first energy polymorph of **5a** for cocrystal form.

```
data_00405_-4.81214E+01
_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                17.491
_cell_length_b                5.834
```

_cell_length_c 8.997
_cell_angle_alpha 90.00
_cell_angle_beta 126.42
_cell_angle_gamma 90.00
_cell_volume 738.764
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.52887 0.30140 0.24648
H*2 H 0.58047 0.22464 0.24411
H*3 H 0.46552 0.23633 0.13830
H*4 H 0.53814 0.24811 0.36407
N'1+ N 0.04949 0.27143 0.69776
N'2+ N 0.20296 0.20806 0.92571
N3+ N 0.11600 0.22786 0.87430
N'4+ N 0.09551 0.28205 0.62308
C5+ C 0.18807 0.24348 0.76231
C6+ C 0.26407 0.24006 0.74019
N'7+ N 0.24918 0.27548 0.57679
N8+ N 0.33614 0.25568 0.62820
N'9+ N 0.40265 0.21211 0.80474
N'10+ N 0.35663 0.20149 0.87942
O11+ O 0.09682 0.20395 0.99945
O12+ O 0.35532 0.27959 0.50305
H*13+ H 0.02837 0.22615 0.92703
H*14+ H 0.42377 0.25739 0.57547

#END

S98. Optimized crystal structure coordinates for first energy polymorph of **5b** for cocrystal form.

data_01013_-5.83522E+01
_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 4.283
_cell_length_b 16.474
_cell_length_c 5.546
_cell_angle_alpha 90.00
_cell_angle_beta 99.38
_cell_angle_gamma 90.00
_cell_volume 386.083
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x

_atom_site_fract_y
_atom_site_fract_z
N1 N 0.18374 0.70834 0.77543
H*2 H 0.16266 0.65890 0.88294
H*3 H 0.16272 0.75779 0.88298
O4 O -0.10727 0.70836 0.60177
H*5 H -0.03260 0.70836 0.44673
N'1+ N -0.06337 -0.18886 0.25223
N'2+ N -0.21663 -0.05905 0.25778
N3+ N -0.21905 -0.13180 0.35094
N'4+ N 0.05487 -0.15140 0.07673
C5+ C -0.03958 -0.07309 0.08226
C6+ C 0.03952 -0.01019 -0.08224
N'7+ N 0.21657 -0.02423 -0.25776
N8+ N 0.21899 0.04852 -0.35092
N'9+ N 0.06331 0.10558 -0.25221
N'10+ N -0.05493 0.06812 -0.07671
O11+ O -0.37627 -0.14645 0.54055
O12+ O 0.37621 0.06317 -0.54053
H*13+ H -0.34149 -0.20405 0.57430
H*14+ H 0.34143 0.12077 -0.57428

#END

S99. Optimized crystal structure coordinates for first energy polymorph of **5c** for cocrystal form.

data_07574_-5.07475E+01
_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 8.775
_cell_length_b 20.832
_cell_length_c 4.858
_cell_angle_alpha 90.00
_cell_angle_beta 119.63
_cell_angle_gamma 90.00
_cell_volume 771.922
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.35846 -0.24727 0.65464
H*2 H -0.36779 -0.28530 0.51484
H*3 H -0.28507 -0.26133 0.88415
N4 N -0.52685 -0.22771 0.60690

H*5 H -0.57603 -0.19457 0.43012
H*6 H -0.61322 -0.26504 0.53833
N'1+ N -0.73153 0.58643 -0.11634
N'2+ N -0.48760 0.64458 0.16047
N3+ N -0.64769 0.63182 0.09559
N'4+ N -0.61816 0.56672 -0.20252
C5+ C -0.47153 0.60225 -0.03350
C6+ C -0.31275 0.59599 -0.05612
N'7+ N -0.29668 0.55366 -0.25009
N8+ N -0.13659 0.56642 -0.18521
N'9+ N -0.05275 0.61181 0.02672
N'10+ N -0.16612 0.63152 0.11290
O11+ O -0.72139 0.66445 0.24273
O12+ O -0.06289 0.53379 -0.33235
H*13+ H -0.83841 0.64611 0.15387
H*14+ H 0.05413 0.55213 -0.24349

#END

S100. Optimized crystal structure coordinates for first energy polymorph of **5d** for cocrystal form.

data_00745_-6.64945E+01
_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 7.704
_cell_length_b 17.017
_cell_length_c 6.718
_cell_angle_alpha 90.00
_cell_angle_beta 91.72
_cell_angle_gamma 90.00
_cell_volume 880.326
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.25808 0.67504 0.11964
N'2 N -0.34150 0.73586 0.05603
H*3 H -0.26909 0.78570 0.07399
N4 N -0.34090 0.60235 0.12908
H*5 H -0.26808 0.55585 0.08774
H*6 H -0.46023 0.60330 0.06151
N7 N -0.08377 0.67120 0.18349
H*8 H -0.02616 0.72413 0.20378

H*9 H -0.05800 0.63337 0.29714
N'1+ N -0.33881 0.11531 0.60660
N'2+ N -0.10848 0.17971 0.73583
N3+ N -0.26643 0.18279 0.66008
N'4+ N -0.21926 0.06183 0.64999
C5+ C -0.08097 0.10157 0.72787
C6+ C 0.08077 0.06475 0.79625
N'7+ N 0.10828 -0.01339 0.78829
N8+ N 0.26623 -0.01647 0.86404
N'9+ N 0.33861 0.05101 0.91752
N'10+ N 0.21906 0.10449 0.87413
O11+ O -0.34945 0.25293 0.63895
O12+ O 0.34925 -0.08661 0.88517
H*13+ H -0.46250 0.23909 0.58037
H*14+ H 0.46230 -0.07277 0.94375

#END

S101. Optimized crystal structure coordinates for first energy polymorph of **5e** for cocrystal form.

data_08109_-6.50001E+01
_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 6.200
_cell_length_b 10.838
_cell_length_c 15.409
_cell_angle_alpha 90.00
_cell_angle_beta 95.28
_cell_angle_gamma 90.00
_cell_volume 1031.02
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.89587 0.24839 -0.14528
N2 N 0.85110 0.13702 -0.10527
H*3 H 0.82775 0.14551 -0.04124
N'4 N 1.05016 0.25281 -0.19627
N5 N 0.76597 0.34635 -0.12524
H*6 H 0.61278 0.32232 -0.11446
H*7 H 0.77517 0.41665 -0.16853
N8 N 1.05753 0.37147 -0.23924
H*9 H 1.17503 0.42228 -0.20470

H*10 H 1.11801 0.35369 -0.29719
H*11 H 0.96347 0.07185 -0.11544
N'1+ N 0.12612 0.38444 0.05027
N'2+ N 0.42005 0.31395 -0.00797
N3+ N 0.26141 0.39354 -0.01088
N'4+ N 0.19970 0.29036 0.09885
C5+ C 0.37715 0.24875 0.06292
C6+ C 0.50897 0.14499 0.09642
N'7+ N 0.46607 0.07979 0.16731
N8+ N 0.62471 0.00020 0.17022
N'9+ N 0.76000 0.00930 0.10907
N'10+ N 0.68642 0.10338 0.06049
O11+ O 0.24031 0.48070 -0.07455
O12+ O 0.64581 -0.08696 0.23389
H*13+ H 0.11220 0.52705 -0.06208
H*14+ H 0.77392 -0.13331 0.22142

#END

S102. Optimized crystal structure coordinates for first energy polymorph of **5f** for cocrystal form.

data_09724_-6.19246E+01
_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 14.840
_cell_length_b 14.167
_cell_length_c 5.768
_cell_angle_alpha 90.00
_cell_angle_beta 116.10
_cell_angle_gamma 90.00
_cell_volume 1089
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.20543 0.72585 0.06879
N'2 N 0.14807 0.70068 0.17358
N3 N 0.22121 0.66464 -0.09991
H*4 H 0.29331 0.66460 -0.07448
N5 N 0.25721 0.81061 0.11138
N6 N 0.18378 0.57111 -0.12760
N7 N 0.13532 0.77556 0.32607
H*8 H 0.19325 0.77145 0.50770

H*9 H 0.18275 0.55147 0.04203
H*10 H 0.11050 0.57331 -0.26048
H*11 H 0.07287 0.75802 0.34716
H*12 H 0.26701 0.83393 -0.04217
H*13 H 0.22699 0.86011 0.18428
N'1+ N 0.51017 0.39292 0.45454
N'2+ N 0.62237 0.34456 0.31824
N3+ N 0.58014 0.41467 0.38040
N'4+ N 0.50455 0.29985 0.44139
C5+ C 0.57270 0.27166 0.35885
C6+ C 0.59120 0.17354 0.31751
N'7+ N 0.54153 0.10064 0.35812
N8+ N 0.58376 0.03053 0.29596
N'9+ N 0.65373 0.05228 0.22182
N'10+ N 0.65935 0.14535 0.23497
O11+ O 0.60830 0.50510 0.36766
O12+ O 0.55560 -0.05990 0.30870
H*13+ H 0.56629 0.54273 0.42278
H*14+ H 0.59761 -0.09753 0.25358

#END

S103. Optimized crystal structure coordinates for first energy polymorph of **5g** for cocrystal form.

data_09637_-6.31697E+01
_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 10.560
_cell_length_b 12.138
_cell_length_c 8.764
_cell_angle_alpha 90.00
_cell_angle_beta 95.86
_cell_angle_gamma 90.00
_cell_volume 1117.48
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.74948 0.61855 -0.21371
N'2 N 0.68194 0.65274 -0.10749
N3 N 0.61260 0.56360 -0.04527
N4 N 0.76029 0.50775 -0.25214
N5 N 0.81115 0.48378 -0.39194

N6 N 0.81641 0.69310 -0.29347
N7 N 0.83689 0.80090 -0.23534
H*8 H 0.54705 0.60076 0.01475
H*9 H 0.67289 0.52304 0.03484
H*10 H 0.68093 0.46555 -0.22888
H*11 H 0.85761 0.41054 -0.38007
H*12 H 0.74104 0.47839 -0.48073
H*13 H 0.89009 0.66158 -0.34440
H*14 H 0.75429 0.84346 -0.26143
H*15 H 0.84784 0.79675 -0.11801
N'1+ N 0.53894 0.21040 0.39406
N'2+ N 0.59721 0.38671 0.37393
N3+ N 0.52290 0.31475 0.43065
N'4+ N 0.63238 0.21187 0.30468
C5+ C 0.66659 0.31884 0.29356
C6+ C 0.76717 0.35764 0.20492
N'7+ N 0.83655 0.28977 0.12455
N8+ N 0.91086 0.36173 0.06783
N'9+ N 0.89482 0.46608 0.10442
N'10+ N 0.80138 0.46461 0.19380
O11+ O 0.43401 0.34792 0.52269
O12+ O 0.99975 0.32856 -0.02421
H*13+ H 0.39249 0.27980 0.54871
H*14+ H 1.04127 0.39668 -0.05023

#END

S104. Optimized crystal structure coordinates for first energy polymorph of **6a** for cocrystal form.

data_00158_-4.24926E+01
_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 13.629
_cell_length_b 8.423
_cell_length_c 6.468
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 90.00
_cell_volume 742.507
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z

N1 N 0.44731 0.04459 0.52807
H*2 H 0.45470 -0.06302 0.45775
H*3 H 0.51551 0.09395 0.53435
H*4 H 0.40635 0.11381 0.43190
N'1+ N -0.04361 -0.20029 0.56766
N'2+ N -0.05447 0.06556 0.55571
N3+ N -0.09665 -0.07227 0.59397
N'4+ N 0.04259 -0.14516 0.50586
C5+ C 0.03504 0.01513 0.49932
C6+ C 0.11728 0.11244 0.43713
N7+ N 0.20493 0.04877 0.38295
N'8+ N 0.26726 0.16330 0.33286
N'9+ N 0.21823 0.29625 0.35612
N'10+ N 0.12562 0.26915 0.42019
O11+ O -0.19095 -0.08501 0.65813
O12+ O 0.23389 -0.10607 0.37473
H*13+ H -0.21408 0.02424 0.66575
H*14+ H 0.17547 -0.16694 0.41831

#END

S105. Optimized crystal structure coordinates for first energy polymorph of **6b** for cocrystal form.

data_02996_-5.24504E+01
_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 13.041
_cell_length_b 5.092
_cell_length_c 14.249
_cell_angle_alpha 90.00
_cell_angle_beta 123.51
_cell_angle_gamma 90.00
_cell_volume 788.933
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.53204 0.24914 -0.04520
H*2 H 0.58397 0.08898 -0.00166
H*3 H 0.58431 0.40888 -0.00159
O4 O 0.43497 0.24980 -0.02493
H*5 H 0.36162 0.25006 -0.10012
N'1+ N -0.18066 -0.39581 0.72642

N'2+ N -0.20838 -0.08526 0.60254
N3+ N -0.25446 -0.27861 0.62982
N'4+ N -0.07456 -0.27156 0.76908
C5+ C -0.09254 -0.08500 0.69362
C6+ C 0.00633 0.08699 0.71490
N7+ N 0.12051 0.07015 0.81029
N'8+ N 0.19331 0.24927 0.80872
N'9+ N 0.12432 0.37507 0.71308
N'10+ N 0.00864 0.28002 0.65328
O11+ O -0.37303 -0.35763 0.56248
O12+ O 0.16528 -0.09541 0.89993
H*13+ H -0.40803 -0.24266 0.49715
H*14+ H 0.09462 -0.20771 0.88123

#END

S106. Optimized crystal structure coordinates for first energy polymorph of **6c** for cocrystal form.

data_00155_-4.69466E+01
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'C 2/c'
_symmetry_Int_Tables_number 15
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z
_cell_length_a 12.486
_cell_length_b 7.277
_cell_length_c 17.582
_cell_angle_alpha 90.00
_cell_angle_beta 76.41
_cell_angle_gamma 90.00
_cell_volume 1552.78
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.67923 -0.07511 0.06807
H*2 H 0.69574 0.05842 0.05182
H*3 H 0.60763 -0.07755 0.11002
N4 N 0.76351 -0.15405 0.10117
H*5 H 0.82131 -0.20978 0.05660
H*6 H 0.80154 -0.05769 0.12779
N'1+ N 0.00129 0.05837 0.63428

N'2+ N 0.15929 0.16350 0.55769
N3+ N 0.05172 0.14189 0.56984
N'4+ N 0.08152 0.01933 0.66938
C5+ C 0.17624 0.08339 0.62262
C6+ C 0.28033 0.06256 0.64428
N7+ N 0.28813 -0.02112 0.71164
N'8+ N 0.39215 -0.02193 0.71727
N'9+ N 0.44777 0.06063 0.65384
N'10+ N 0.38138 0.11438 0.60763
O11+ O -0.00672 0.20207 0.51886
O12+ O 0.20825 -0.09791 0.76930
H*13+ H 0.04818 0.25812 0.47662
H*14+ H 0.13940 -0.08009 0.75173

#END

S107. Optimized crystal structure coordinates for first energy polymorph of **6d** for cocrystal form.

data_04631_-6.02880E+01
_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 13.184
_cell_length_b 11.297
_cell_length_c 6.670
_cell_angle_alpha 90.00
_cell_angle_beta 112.97
_cell_angle_gamma 90.00
_cell_volume 914.658
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.42694 0.13909 0.11196
N'2 N 0.35450 0.12764 -0.08298
H*3 H 0.34276 0.04082 -0.12841
N4 N 0.46395 0.25117 0.19634
H*5 H 0.47502 0.26274 0.35423
H*6 H 0.41896 0.31655 0.09756
N7 N 0.47651 0.04884 0.26193
H*8 H 0.46295 -0.03364 0.19785
H*9 H 0.55641 0.06314 0.36060
N'1+ N -0.27760 1.01424 -0.45836
N'2+ N -0.16258 1.07586 -0.12751

N3+ N -0.22841 1.10218 -0.32915
N'4+ N -0.24227 0.91921 -0.33405
C5+ C -0.17305 0.95758 -0.13520
C6+ C -0.11977 0.87506 0.04019
N7+ N -0.13629 0.75665 0.01450
N'8+ N -0.07805 0.70151 0.19924
N'9+ N -0.02619 0.78547 0.33723
N'10+ N -0.05006 0.89341 0.24450
O11+ O -0.24621 1.21479 -0.40471
O12+ O -0.20035 0.69317 -0.16393
H*13+ H -0.20137 1.26287 -0.28051
H*14+ H -0.23458 0.75329 -0.27804

#END

S108. Optimized crystal structure coordinates for first energy polymorph of **6e** for cocrystal form.

data_10064_-6.10610E+01
_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 7.076
_cell_length_b 14.105
_cell_length_c 12.700
_cell_angle_alpha 90.00
_cell_angle_beta 51.59
_cell_angle_gamma 90.00
_cell_volume 993.232
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.73803 -0.08912 0.63871
N2 N 0.81318 -0.08253 0.50814
H*3 H 0.98469 -0.10511 0.43667
N'4 N 0.62237 -0.01898 0.72066
N5 N 0.79804 -0.17312 0.66790
H*6 H 0.80074 -0.23057 0.61908
H*7 H 0.69941 -0.18204 0.76889
N8 N 0.53593 -0.04238 0.85508
H*9 H 0.65700 -0.01461 0.86552
H*10 H 0.38359 -0.00305 0.91764
H*11 H 0.78527 -0.01659 0.48833
N'1+ N 0.45024 0.26189 0.06010

N'2+ N 0.66283 0.39721 -0.02144
N3+ N 0.50586 0.34360 0.08333
N'4+ N 0.58082 0.25934 -0.07242
C5+ C 0.70802 0.34127 -0.12029
C6+ C 0.87013 0.36096 -0.26282
N7+ N 0.90238 0.29912 -0.35446
N'8+ N 1.05949 0.33422 -0.47718
N'9+ N 1.12317 0.41697 -0.46098
N'10+ N 1.00987 0.43562 -0.33017
O11+ O 0.40297 0.36993 0.21117
O12+ O 0.80069 0.21248 -0.33655
H*13+ H 0.47206 0.43199 0.20206
H*14+ H 0.69247 0.20257 -0.23827

#END

S109. Optimized crystal structure coordinates for first energy polymorph of **6f** for cocrystal form.

data_07034_-5.74601E+01
_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 4.401
_cell_length_b 22.329
_cell_length_c 10.761
_cell_angle_alpha 90.00
_cell_angle_beta 76.48
_cell_angle_gamma 90.00
_cell_volume 1028.18
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.06420 -0.17178 0.39324
N'2 N -0.01839 -0.15865 0.51338
N3 N 0.05608 -0.12793 0.30136
H*4 H -0.02460 -0.14368 0.22672
N5 N 0.15931 -0.22779 0.34294
N6 N -0.08036 -0.07161 0.34223
N7 N 0.02728 -0.20834 0.59276
H*8 H -0.16927 -0.23442 0.60844
H*9 H -0.24917 -0.07788 0.42452
H*10 H 0.08799 -0.04642 0.36792
H*11 H 0.02855 -0.19005 0.67921

H*12 H 0.31582 -0.22653 0.25728
H*13 H 0.22934 -0.25394 0.40854
N'1+ N 0.59996 0.52196 0.18520
N'2+ N 0.36613 0.61104 0.23464
N3+ N 0.41812 0.56403 0.15839
N'4+ N 0.67955 0.54195 0.28911
C5+ C 0.53713 0.59564 0.31787
C6+ C 0.57640 0.62973 0.42725
N7+ N 0.75556 0.60985 0.50546
N'8+ N 0.75188 0.64938 0.59771
N'9+ N 0.57182 0.69317 0.57628
N'10+ N 0.45993 0.68249 0.47201
O11+ O 0.29202 0.55814 0.05563
O12+ O 0.92452 0.55836 0.50063
H*13+ H 0.16890 0.59442 0.05617
H*14+ H 0.88986 0.53692 0.42482

#END

S110. Optimized crystal structure coordinates for first energy polymorph of **6g** for cocrystal form.

data_05338_-6.12915E+01
_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 7.288
_cell_length_b 20.978
_cell_length_c 8.907
_cell_angle_alpha 90.00
_cell_angle_beta 124.84
_cell_angle_gamma 90.00
_cell_volume 1117.67
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.51407 0.33358 0.21451
N'2 N 0.40850 0.28700 0.22958
N3 N 0.23514 0.30995 0.24758
N4 N 0.45263 0.39728 0.20254
N5 N 0.60999 0.44384 0.22995
N6 N 0.69496 0.32114 0.20724
N7 N 0.73054 0.25848 0.17087
H*8 H 0.19146 0.27167 0.29071

H*9 H 0.09682 0.32037 0.11970
H*10 H 0.37516 0.40403 0.26714
H*11 H 0.52473 0.48282 0.15409
H*12 H 0.71258 0.45668 0.36423
H*13 H 0.73331 0.35571 0.15041
H*14 H 0.80059 0.23334 0.28953
H*15 H 0.57791 0.23757 0.08242
N'1+ N -0.16129 0.57529 0.42619
N'2+ N -0.15623 0.65417 0.25816
N3+ N -0.22537 0.63259 0.35694
N'4+ N -0.03718 0.55591 0.36975
C5+ C -0.03551 0.60388 0.26869
C6+ C 0.08629 0.59792 0.18614
N7+ N 0.20341 0.54467 0.20563
N'8+ N 0.29883 0.55157 0.11688
N'9+ N 0.24070 0.60863 0.04350
N'10+ N 0.10979 0.63846 0.08350
O11+ O -0.35753 0.66712 0.38813
O12+ O 0.23195 0.48958 0.29796
H*13+ H -0.38144 0.70708 0.32365
H*14+ H 0.14606 0.49613 0.35130

#END

S111. Optimized crystal structure coordinates for first energy polymorph of **7a** for cocrystal form.

data_NH3_BTO_0_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 12.595
_cell_length_b 5.942
_cell_length_c 9.963
_cell_angle_alpha 90.00
_cell_angle_beta 95.31
_cell_angle_gamma 90.00
_cell_volume 742.426
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.16579 0.74773 0.49114
H*2 H -0.23890 0.67439 0.47366
H*3 H -0.15956 0.86251 0.41627

H*4 H -0.16615 0.83585 0.57885
N1 N 0.16580 0.25228 0.00887
H*2 H 0.23891 0.32562 0.02636
H*3 H 0.16617 0.16415 -0.07884
H*4 H 0.15957 0.13750 0.08374
N'1+ N 0.36639 0.37102 0.31333
N'2+ N 0.43176 0.21523 0.13939
N'3+ N 0.37046 0.38268 0.18396
N4+ N 0.42621 0.19219 0.35565
C5+ C 0.46592 0.09794 0.24784
C6+ C 0.53408 -0.09794 0.25216
N'7+ N 0.56824 -0.21523 0.36061
N'8+ N 0.62954 -0.38268 0.31604
N'9+ N 0.63361 -0.37102 0.18667
N10+ N 0.57379 -0.19219 0.14435
H*11+ H 0.43617 0.14596 0.45392
H*12+ H 0.56383 -0.14596 0.04608

#END

S112. Optimized crystal structure coordinates for first energy polymorph of **7b** for cocrystal form.

data_NH2OH_BTO_0_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 11.754
_cell_length_b 5.012
_cell_length_c 6.984
_cell_angle_alpha 96.82
_cell_angle_beta 89.80
_cell_angle_gamma 95.03
_cell_volume 406.94
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.56570 0.25099 -0.07970
H*2 H 0.53281 0.39432 -0.15054
H*3 H 0.53368 0.06957 -0.15000
O4 O 0.50663 0.26872 0.10266
H*5 H 0.56863 0.29795 0.19509
N1 N -0.06571 0.24899 0.57968
H*2 H -0.03370 0.43040 0.65002
H*3 H -0.03282 0.10565 0.65051
O4 O -0.00662 0.23132 0.39734

H*5 H -0.06861 0.20209 0.30490
N'1+ N -0.35973 0.52191 -0.60736
N'2+ N -0.32081 0.91376 -0.43492
N'3+ N -0.36956 0.77869 -0.59864
N4+ N -0.30331 0.48548 -0.44619
C5+ C -0.27988 0.72775 -0.34147
C6+ C -0.22012 0.77229 -0.15855
N'7+ N -0.17919 0.58628 -0.06510
N'8+ N -0.13044 0.72135 0.09862
N'9+ N -0.14027 0.97813 0.10734
N10+ N -0.19669 1.01456 -0.05383
H*11+ H -0.28448 0.30058 -0.41780
H*12+ H -0.21552 1.19946 -0.08222

#END

S113. Optimized crystal structure coordinates for first energy polymorph of **7c** for cocrystal form.

data_N2H4_BTO_0_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 6.734
_cell_length_b 9.948
_cell_length_c 7.735
_cell_angle_alpha 121.67
_cell_angle_beta 95.46
_cell_angle_gamma 93.18
_cell_volume 435.591
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.77591 -0.09886 0.18312
H*2 H -0.66113 -0.08617 0.11375
H*3 H -0.75161 -0.00749 0.33259
N4 N -0.78254 -0.24474 0.17997
H*5 H -0.87101 -0.33012 0.04829
H*6 H -0.64376 -0.28112 0.17902
N1 N 0.22405 0.40112 0.18311
H*2 H 0.33881 0.41382 0.11371
H*3 H 0.24837 0.49251 0.33258
N4 N 0.21746 0.25525 0.17997
H*5 H 0.12898 0.16986 0.04831
H*6 H 0.35625 0.21888 0.17901
N'1+ N -0.36628 0.06777 0.22960

N'2+ N -0.20447 0.30843 0.38566
N'3+ N -0.37066 0.20838 0.25900
N4+ N -0.19369 0.07445 0.33891
C5+ C -0.09566 0.22293 0.43407
C6+ C 0.09566 0.27707 0.56593
N'7+ N 0.20447 0.19157 0.61434
N'8+ N 0.37066 0.29162 0.74100
N'9+ N 0.36628 0.43223 0.77040
N10+ N 0.19369 0.42555 0.66109
H*11+ H -0.15383 -0.02112 0.34196
H*12+ H 0.15383 0.52112 0.65804

#END

S114. Optimized crystal structure coordinates for first energy polymorph of **7d** for cocrystal form.

data_G_BTO_0_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 8.649
_cell_length_b 9.334
_cell_length_c 8.330
_cell_angle_alpha 66.78
_cell_angle_beta 84.67
_cell_angle_gamma 61.80
_cell_volume 541.016
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.59864 0.32144 -0.20365
N'2 N 0.52137 0.46864 -0.18401
H*3 H 0.45131 0.45986 -0.07821
N4 N 0.68500 0.31116 -0.35177
H*5 H 0.80099 0.19857 -0.32851
H*6 H 0.69417 0.42264 -0.42397
N7 N 0.61020 0.15889 -0.08882
H*8 H 0.53014 0.16636 0.00750
H*9 H 0.60665 0.08372 -0.14766
C1 C 0.09863 -0.17854 0.79636
N'2 N 0.02135 -0.03134 0.81600
H*3 H -0.04872 -0.04012 0.92179
N4 N 0.18500 -0.18882 0.64824
H*5 H 0.30100 -0.30140 0.67150
H*6 H 0.19416 -0.07733 0.57604

N7 N 0.11021 -0.34109 0.91119
H*8 H 0.03015 -0.33363 1.00751
H*9 H 0.10668 -0.41627 0.85235
N'1+ N 0.10105 0.31469 0.80367
N'2+ N 0.22928 0.41590 0.58045
N'3+ N 0.15493 0.43118 0.72789
N4+ N 0.14036 0.22003 0.70463
C5+ C 0.21909 0.28352 0.56790
C6+ C 0.28089 0.21646 0.43212
N'7+ N 0.27070 0.08408 0.41957
N'8+ N 0.34505 0.06880 0.27213
N'9+ N 0.39893 0.18529 0.19635
N10+ N 0.35962 0.27995 0.29539
H*11+ H 0.11159 0.11947 0.73577
H*12+ H 0.38839 0.38051 0.26425

#END

S115. Optimized crystal structure coordinates for first energy polymorph of **7e** for cocrystal form.

data_AGXR_BTO_0_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 13.521
_cell_length_b 10.750
_cell_length_c 9.308
_cell_angle_alpha 90.00
_cell_angle_beta 97.88
_cell_angle_gamma 90.00
_cell_volume 1340.15
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.41603 0.70171 0.05557
N2 N 0.33924 0.78142 -0.00180
H*3 H 0.28186 0.73773 -0.06341
N'4 N 0.50770 0.73396 0.05090
N5 N 0.38488 0.59208 0.11328
H*6 H 0.32111 0.59978 0.15845
H*7 H 0.44204 0.55034 0.17822
N8 N 0.57702 0.64688 0.12929
H*9 H 0.59971 0.58776 0.05415

H*10 H 0.63870 0.69811 0.16587
H*11 H 0.36560 0.85417 -0.05469
C1 C 0.08392 0.20163 0.44434
N2 N 0.16072 0.28132 0.50173
H*3 H 0.21809 0.23760 0.56332
N'4 N -0.00775 0.23389 0.44903
N5 N 0.11504 0.09201 0.38657
H*6 H 0.17881 0.09972 0.34140
H*7 H 0.05788 0.05031 0.32163
N8 N -0.07709 0.14684 0.37061
H*9 H -0.09978 0.08771 0.44573
H*10 H -0.13876 0.19810 0.33406
H*11 H 0.13437 0.35405 0.55465
N'1+ N -0.18021 0.35930 0.16952
N'2+ N -0.12083 0.50543 0.32148
N'3+ N -0.20040 0.43248 0.27233
N4+ N -0.08529 0.38408 0.14991
C5+ C -0.04966 0.47401 0.24392
C6+ C 0.04966 0.52599 0.25614
N'7+ N 0.12083 0.49458 0.17858
N'8+ N 0.20040 0.56752 0.22773
N'9+ N 0.18021 0.64070 0.33054
N10+ N 0.08529 0.61592 0.35015
H*11+ H -0.05110 0.33889 0.07480
H*12+ H 0.05110 0.66111 0.42526

#END

S116. Optimized crystal structure coordinates for first energy polymorph of **7f** for cocrystal form.

data_DAGXR_BTO_0_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 10.285
_cell_length_b 10.290
_cell_length_c 6.830
_cell_angle_alpha 95.01
_cell_angle_beta 72.97
_cell_angle_gamma 96.92
_cell_volume 685.075
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.19675 -0.15197 0.28793

N'2 N 0.26843 -0.03924 0.27042
N3 N 0.11397 -0.19066 0.15907
H*4 H 0.02235 -0.23730 0.23311
N5 N 0.19070 -0.24238 0.43051
N6 N 0.09715 -0.09817 0.02832
N7 N 0.35435 -0.02111 0.40593
H*8 H 0.29818 0.01624 0.54455
H*9 H 0.10659 -0.00636 0.09682
H*10 H 0.17833 -0.10001 -0.09998
H*11 H 0.42734 0.05246 0.34801
H*12 H 0.17421 -0.33704 0.38104
H*13 H 0.27266 -0.22525 0.48731
C1 C 0.19674 0.34802 0.28792
N'2 N 0.26842 0.46075 0.27041
N3 N 0.11396 0.30933 0.15906
H*4 H 0.02234 0.26269 0.23310
N5 N 0.19069 0.25761 0.43050
N6 N 0.09714 0.40182 0.02831
N7 N 0.35434 0.47888 0.40592
H*8 H 0.29817 0.51623 0.54454
H*9 H 0.10658 0.49363 0.09681
H*10 H 0.17832 0.39998 -0.09999
H*11 H 0.42733 0.55245 0.34800
H*12 H 0.17420 0.16295 0.38103
H*13 H 0.27265 0.27473 0.48730
N'1+ N 0.30179 0.13432 -0.20333
N'2+ N 0.44930 0.30779 -0.21304
N'3+ N 0.35286 0.24203 -0.29449
N4+ N 0.36555 0.12832 -0.05832
C5+ C 0.45592 0.23547 -0.06587
C6+ C 0.54410 0.26453 0.06583
N'7+ N 0.55072 0.19221 0.21300
N'8+ N 0.64716 0.25797 0.29445
N'9+ N 0.69823 0.36568 0.20329
N10+ N 0.63447 0.37168 0.05828
H*11+ H 0.34393 0.05274 0.03552
H*12+ H 0.65609 0.44726 -0.03556

#END

S117. Optimized crystal structure coordinates for first energy polymorph of **7g** for cocrystal form.

data_TAGXR_BTO_0_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 11.859
_cell_length_b 10.752

_cell_length_c 6.597
_cell_angle_alpha 83.42
_cell_angle_beta 68.80
_cell_angle_gamma 72.94
_cell_volume 749.701
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.21208 -0.02062 0.51652
N'2 N 0.29426 0.04546 0.46610
N3 N 0.37174 0.03238 0.23901
N4 N 0.19572 -0.08664 0.36377
N5 N 0.12523 -0.17884 0.44452
N6 N 0.13444 -0.02656 0.72975
N7 N 0.12265 0.06338 0.88133
H*8 H 0.44531 0.06698 0.22537
H*9 H 0.32356 0.09566 0.15084
H*10 H 0.27757 -0.11346 0.23521
H*11 H 0.08086 -0.18195 0.34000
H*12 H 0.18184 -0.26923 0.45675
H*13 H 0.05414 -0.04964 0.75112
H*14 H 0.20070 0.03204 0.92478
H*15 H 0.12870 0.15018 0.80222
C1 C 0.21208 0.47937 0.51652
N'2 N 0.29426 0.54545 0.46610
N3 N 0.37174 0.53237 0.23901
N4 N 0.19572 0.41335 0.36377
N5 N 0.12523 0.32115 0.44452
N6 N 0.13444 0.47343 0.72975
N7 N 0.12265 0.56337 0.88133
H*8 H 0.44531 0.56697 0.22537
H*9 H 0.32356 0.59565 0.15084
H*10 H 0.27757 0.38653 0.23521
H*11 H 0.08086 0.31804 0.34000
H*12 H 0.18184 0.23076 0.45675
H*13 H 0.05414 0.45035 0.75112
H*14 H 0.20070 0.53203 0.92478
H*15 H 0.12870 0.65017 0.80222
N'1+ N 0.31060 0.21711 0.90783
N'2+ N 0.44911 0.32865 0.76505
N'3+ N 0.35723 0.30321 0.94603
N4+ N 0.37273 0.18464 0.69718
C5+ C 0.45756 0.25384 0.61130
C6+ C 0.54244 0.24616 0.38868
N'7+ N 0.55089 0.17135 0.23493
N'8+ N 0.64277 0.19679 0.05395
N'9+ N 0.68940 0.28289 0.09215
N10+ N 0.62727 0.31536 0.30280
H*11+ H 0.35383 0.11832 0.62585

H*12+ H 0.64617 0.38168 0.37413

#END

S118. Optimized crystal structure coordinates for first energy polymorph of **8a** for cocrystal form.

data_NH3_BTO_1_1
_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M 'P 21/a'
_symmetry_Int_Tables_number 14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,1/2+y,-z
3 -x,-y,-z
4 1/2+x,1/2-y,z
_cell_length_a 15.001
_cell_length_b 7.580
_cell_length_c 6.999
_cell_angle_alpha 90.00
_cell_angle_beta 96.66
_cell_angle_gamma 90.00
_cell_volume 790.469
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.62098 0.52634 0.14969
H*2 H 0.66414 0.46494 0.25170
H*3 H 0.56112 0.53731 0.20427
H*4 H 0.64460 0.65121 0.13598
N1 N 0.05840 0.37909 0.28257
H*2 H 0.10666 0.44444 0.36962
H*3 H 0.01259 0.47094 0.22883
H*4 H 0.08819 0.33188 0.16930
N'1+ N 0.06509 0.32815 0.80185
N2+ N 0.18808 0.19238 0.83975
N'3+ N 0.14834 0.34096 0.88291
N'4+ N 0.05075 0.17387 0.70741
C5+ C 0.12863 0.08860 0.73178
C6+ C 0.15299 -0.08164 0.66343
N7+ N 0.10142 -0.19788 0.55590
N'8+ N 0.15209 -0.34078 0.52550
N'9+ N 0.23134 -0.31036 0.61231
N'10+ N 0.23460 -0.15009 0.70003
O11+ O 0.27601 0.16246 0.90238
H*12+ H 0.28850 0.04432 0.85101
H*13+ H 0.03589 -0.18967 0.50178

#END

S119. Optimized crystal structure coordinates for first energy polymorph of **8b** for cocrystal form.

```
data_NH2OH_BTO_1_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                 6.970
_cell_length_b                 11.801
_cell_length_c                 6.968
_cell_angle_alpha               107.57
_cell_angle_beta                117.95
_cell_angle_gamma               102.71
_cell_volume                   435.935
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.23515 -0.11963 0.35623
H*2 H -0.34723 -0.19918 0.34133
H*3 H -0.26357 -0.04191 0.43203
O4 O -0.34143 -0.14407 0.10458
H*5 H -0.21017 -0.13920 0.08829
N1 N 0.59305 0.40444 0.09482
H*2 H 0.49614 0.32107 0.08400
H*3 H 0.54976 0.47543 0.16699
O4 O 0.47854 0.37750 -0.15888
H*5 H 0.61066 0.39146 -0.17528
N'1+ N -0.15483 -0.33701 0.85455
N2+ N 0.05813 -0.17055 0.87576
N'3+ N -0.06279 -0.20781 0.96330
N'4+ N -0.09500 -0.38326 0.69871
C5+ C 0.03952 -0.27773 0.71278
C6+ C 0.15305 -0.26737 0.58775
N7+ N 0.14994 -0.36449 0.42273
N'8+ N 0.28097 -0.30962 0.35308
N'9+ N 0.35950 -0.18377 0.47304
N'10+ N 0.28359 -0.15350 0.62134
O11+ O 0.17697 -0.04094 0.95146
H*12+ H 0.25054 -0.04049 0.85955
H*13+ H 0.06840 -0.46329 0.35363

#END
```

S120. Optimized crystal structure coordinates for first energy polymorph of **8c** for cocrystal form.

```
data_N2H4_BTO_1_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                 8.642
_cell_length_b                 8.206
_cell_length_c                 14.560
_cell_angle_alpha               90.00
_cell_angle_beta                64.12
_cell_angle_gamma                 90.00
_cell_volume                   928.987
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.14791 0.14205 -0.33331
H*2 H -0.04610 0.08723 -0.32808
H*3 H -0.20494 0.05791 -0.35977
N4 N -0.09494 0.27576 -0.40410
H*5 H -0.09436 0.37779 -0.36464
H*6 H 0.02635 0.25985 -0.46070
N1 N 0.69410 0.70539 0.31584
H*2 H 0.77931 0.72183 0.24130
H*3 H 0.74032 0.61497 0.34473
N4 N 0.52786 0.65530 0.32637
H*5 H 0.45808 0.75774 0.33202
H*6 H 0.53575 0.59135 0.26439
N'1+ N 0.07545 -0.40811 0.60574
N2+ N 0.15886 -0.18259 0.63617
N'3+ N 0.02193 -0.26054 0.63986
N'4+ N 0.24440 -0.42615 0.58022
C5+ C 0.29648 -0.28336 0.59958
C6+ C 0.46357 -0.23173 0.58709
N7+ N 0.61047 -0.31788 0.55196
N'8+ N 0.73618 -0.22073 0.55327
N'9+ N 0.66609 -0.08115 0.58810
N'10+ N 0.49619 -0.08313 0.61008
O11+ O 0.14798 -0.02461 0.66660
H*12+ H 0.26605 0.00337 0.65621
H*13+ H 0.63338 -0.43491 0.52747

#END
```

S121. Optimized crystal structure coordinates for first energy polymorph of **8d** for cocrystal form.

```
data_G_BTO_1_1
_symmetry_cell_setting          monoclinic
_symmetry_space_group_name_H-M   'P 21/c'
_symmetry_Int_Tables_number      14
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2+y,1/2-z
3 -x,-y,-z
4 x,1/2-y,1/2+z
_cell_length_a                 9.857
_cell_length_b                 17.520
_cell_length_c                 6.928
_cell_angle_alpha               90.00
_cell_angle_beta                102.35
_cell_angle_gamma                90.00
_cell_volume                   1168.74
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.53819 -0.33165 0.67150
N'2 N 0.43389 -0.30769 0.73825
H*3 H 0.44689 -0.25223 0.78346
N4 N 0.54805 -0.40835 0.62270
H*5 H 0.58408 -0.41802 0.49839
H*6 H 0.45973 -0.43748 0.62570
N7 N 0.65013 -0.28852 0.63717
H*8 H 0.65616 -0.23526 0.69482
H*9 H 0.74286 -0.31592 0.66440
C1 C -0.04077 0.16766 0.71073
N'2 N 0.06029 0.18570 0.62937
H*3 H 0.05254 0.24096 0.58171
N4 N -0.05801 0.09235 0.76599
H*5 H -0.08708 0.08609 0.89686
H*6 H 0.02398 0.05912 0.75434
N7 N -0.14201 0.21637 0.75608
H*8 H -0.14402 0.26894 0.69514
H*9 H -0.23786 0.19309 0.74099
N'1+ N 0.16118 0.57407 0.37734
N2+ N 0.27776 0.59778 0.16336
N'3+ N 0.23165 0.62839 0.31213
N'4+ N 0.16129 0.50914 0.27293
C5+ C 0.23506 0.52441 0.13796
C6+ C 0.26971 0.47672 -0.01345
N7+ N 0.23478 0.40350 -0.05542
N'8+ N 0.28983 0.38149 -0.20972
N'9+ N 0.35544 0.43985 -0.25792
N'10+ N 0.34533 0.50037 -0.13898
```

O11+ O 0.35570 0.63928 0.06143
H*12+ H 0.37595 0.60356 -0.03966
H*13+ H 0.17784 0.36743 0.00982

#END

S122. Optimized crystal structure coordinates for first energy polymorph of **8e** for cocrystal form.

data_AGXR_BTO_1_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 8.988
_cell_length_b 9.070
_cell_length_c 15.765
_cell_angle_alpha 90.00
_cell_angle_beta 75.47
_cell_angle_gamma 90.00
_cell_volume 1244.08
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.52104 0.52960 0.71659
N2 N 0.38860 0.54921 0.68697
H*3 H 0.29248 0.56714 0.73567
N'4 N 0.61517 0.42435 0.68396
N5 N 0.53827 0.62831 0.78044
H*6 H 0.49486 0.73002 0.77512
H*7 H 0.64833 0.62853 0.78658
N8 N 0.75358 0.43083 0.71516
H*9 H 0.73990 0.35699 0.76556
H*10 H 0.83768 0.38684 0.66602
H*11 H 0.37431 0.46597 0.64676
C1 C -0.00606 0.16832 0.75874
N2 N -0.05067 0.16514 0.85008
H*3 H 0.03840 0.17178 0.87870
N'4 N -0.06752 0.07633 0.71479
N5 N 0.10385 0.27329 0.72335
H*6 H 0.09711 0.36671 0.75936
H*7 H 0.10900 0.29086 0.65891
N8 N -0.02040 0.10632 0.62159
H*9 H 0.06726 0.03506 0.59535
H*10 H -0.10973 0.07206 0.59759

H*11 H -0.11978 0.07769 0.87241
N'1+ N 0.19147 0.08629 0.01996
N2+ N 0.30465 0.25938 -0.05920
N'3+ N 0.17783 0.17842 -0.04197
N'4+ N 0.32490 0.10676 0.04275
C5+ C 0.39596 0.21621 -0.00744
C6+ C 0.54194 0.28476 -0.01169
N7+ N 0.64374 0.25357 0.03530
N'8+ N 0.76532 0.34568 0.00961
N'9+ N 0.73662 0.42902 -0.05079
N'10+ N 0.59838 0.39445 -0.06595
O11+ O 0.32769 0.36709 -0.12115
H*12+ H 0.42913 0.40961 -0.12087
H*13+ H 0.63871 0.17668 0.08258

#END

S123. Optimized crystal structure coordinates for first energy polymorph of **8f** for cocrystal form.

data_DAGXR_BTO_1_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 20.505
_cell_length_b 9.439
_cell_length_c 9.177
_cell_angle_alpha 77.01
_cell_angle_beta 52.71
_cell_angle_gamma 121.78
_cell_volume 714.027
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.37552 0.22199 0.08815
N'2 N 0.44644 0.23155 -0.08692
N3 N 0.36174 0.34309 0.02599
H*4 H 0.37888 0.44534 0.05736
N5 N 0.31087 0.10323 0.34058
N6 N 0.44352 0.50523 -0.25159
N7 N 0.43863 0.07833 0.02676
H*8 H 0.53184 0.21122 -0.05953
H*9 H 0.54301 0.59315 -0.41391
H*10 H 0.37392 0.36889 -0.21102
H*11 H 0.46219 0.04189 -0.07784
H*12 H 0.21568 0.02243 0.50933

H*13 H 0.29111 -0.03411 0.41872
C1 C 0.12561 -0.09701 0.01072
N'2 N 0.23310 0.04441 -0.06979
N3 N 0.12112 0.02743 -0.08865
H*4 H 0.00964 -0.10409 0.07742
N5 N 0.00627 -0.37474 0.19944
N6 N 0.22300 0.29628 -0.24475
N7 N 0.22543 -0.11230 0.03618
H*8 H 0.14650 -0.23084 0.25495
H*9 H 0.24314 0.31713 -0.16726
H*10 H 0.32951 0.43966 -0.47056
H*11 H 0.33272 0.03317 -0.09575
H*12 H -0.02851 -0.42116 0.15169
H*13 H 0.03382 -0.43585 0.20824
N'1+ N 0.66887 0.39005 -0.12535
N2+ N 0.88037 0.68323 -0.36234
N'3+ N 0.82163 0.64690 -0.39744
N'4+ N 0.62861 0.26098 0.08373
C5+ C 0.76262 0.44704 -0.06711
C6+ C 0.79137 0.42516 0.03884
N7+ N 0.68681 0.20565 0.32291
N'8+ N 0.76599 0.27796 0.31800
N'9+ N 0.91306 0.53261 0.03956
N'10+ N 0.93369 0.63178 -0.14150
O11+ O 1.03774 0.93030 -0.60340
H*12+ H 1.04966 0.90189 -0.51618
H*13+ H 0.56826 0.01369 0.51756

#END

S124. Optimized crystal structure coordinates for first energy polymorph of **8g** for cocrystal form.

data_TAGXR_BTO_1_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 10.567
_cell_length_b 7.194
_cell_length_c 12.200
_cell_angle_alpha 67.46
_cell_angle_beta 74.15
_cell_angle_gamma 90.83
_cell_volume 816.573
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y

_atom_site_fract_z
C1 C 0.30408 0.50643 0.86380
N'2 N 0.38255 0.39851 0.92010
N3 N 0.52018 0.48209 0.85495
N4 N 0.34886 0.68884 0.75918
N5 N 0.25932 0.76620 0.69000
N6 N 0.16897 0.44345 0.90806
N7 N 0.11331 0.29214 1.02955
H*8 H 0.57268 0.37030 0.89249
H*9 H 0.54229 0.59745 0.87909
H*10 H 0.44437 0.68961 0.71054
H*11 H 0.27896 0.92015 0.65100
H*12 H 0.26961 0.71473 0.62132
H*13 H 0.11145 0.55330 0.88199
H*14 H 0.13238 0.15609 1.02539
H*15 H 0.16560 0.30994 1.08505
C1 C 0.18243 0.24777 0.55309
N'2 N 0.28627 0.25379 0.58951
N3 N 0.40696 0.32083 0.48622
N4 N 0.18833 0.31434 0.42819
N5 N 0.07492 0.25619 0.40210
N6 N 0.05834 0.17527 0.63961
N7 N 0.03996 0.15550 0.76290
H*8 H 0.48147 0.28585 0.52558
H*9 H 0.41888 0.47622 0.44433
H*10 H 0.27886 0.30030 0.37692
H*11 H 0.06915 0.36683 0.32190
H*12 H 0.08102 0.12233 0.39156
H*13 H -0.01925 0.22062 0.60713
H*14 H 0.07639 0.02621 0.80654
H*15 H 0.10058 0.27071 0.76007
N'1+ N 0.26346 -0.23890 0.44391
N2+ N 0.30726 -0.02448 0.25911
N'3+ N 0.20917 -0.11459 0.36424
N'4+ N 0.39473 -0.23007 0.39166
C5+ C 0.42190 -0.09442 0.27494
C6+ C 0.54550 -0.02344 0.17615
N7+ N 0.66596 -0.07890 0.17851
N'8+ N 0.75372 0.02674 0.06464
N'9+ N 0.68742 0.14144 -0.00328
N'10+ N 0.55722 0.11454 0.06291
O11+ O 0.28475 0.11547 0.15611
H*12+ H 0.37285 0.15800 0.09207
H*13+ H 0.69402 -0.18038 0.24915

#END

S125. Optimized crystal structure coordinates for first energy polymorph of **9a** for cocrystal form.

data_NH3_BTO_2_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2

```
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a                 8.685
_cell_length_b                 9.075
_cell_length_c                 6.628
_cell_angle_alpha               71.00
_cell_angle_beta                110.17
_cell_angle_gamma                 125.49
_cell_volume                   393.848
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N -0.30837 0.25099 0.18746
H*2 H -0.37396 0.18321 0.31806
H*3 H -0.40110 0.27899 0.06269
H*4 H -0.19038 0.37376 0.22680
N1 N 0.36705 0.28042 0.32292
H*2 H 0.24831 0.29011 0.25004
H*3 H 0.33229 0.15726 0.30227
H*4 H 0.47195 0.37953 0.23669
N'1+ N -0.35172 0.16175 0.69803
N'2+ N -0.03963 0.38586 0.74685
N3+ N -0.21930 0.33480 0.72031
N'4+ N -0.25288 0.08939 0.71060
C5+ C -0.06465 0.22625 0.74007
C6+ C 0.09508 0.20560 0.76233
N'7+ N 0.28450 0.34436 0.79201
N'8+ N 0.38374 0.27415 0.80468
N9+ N 0.25426 0.09936 0.78278
N'10+ N 0.07224 0.04839 0.75591
O11+ O -0.26395 0.45676 0.71644
H*12+ H -0.40424 0.38535 0.69509
H*13+ H 0.29243 0.01192 0.78643

#END
```

S126. Optimized crystal structure coordinates for first energy polymorph of **9b** for cocrystal form.

```
data_NH2OH_BTO_2_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 10.539
_cell_length_b 15.296
_cell_length_c 6.595
_cell_angle_alpha 90.00
_cell_angle_beta 125.13
_cell_angle_gamma 90.00
_cell_volume 869.491
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.43285 0.58692 0.04352
H*2 H 0.34226 0.62531 -0.08534
H*3 H 0.50217 0.57994 -0.01745
O4 O 0.36398 0.50147 0.00599
H*5 H 0.39105 0.48701 0.16887
N1 N -0.00909 0.57785 -0.34835
H*2 H -0.08968 0.58896 -0.31172
H*3 H -0.07104 0.56721 -0.53516
O4 O 0.05317 0.49274 -0.24145
H*5 H 0.16314 0.50394 -0.13123
N'1+ N 0.22337 0.14090 -0.29034
N'2+ N 0.38745 0.24961 -0.06440
N3+ N 0.24430 0.22239 -0.21023
N'4+ N 0.36487 0.11031 -0.18981
C5+ C 0.46277 0.17665 -0.05388
C6+ C 0.63129 0.17089 0.08911
N'7+ N 0.72916 0.23811 0.22568
N'8+ N 0.86971 0.20850 0.32612
N9+ N 0.85274 0.12629 0.24893
N'10+ N 0.70724 0.09906 0.10103
O11+ O 0.12462 0.27671 -0.27369
H*12+ H 0.03254 0.24115 -0.38118
H*13+ H 0.94454 0.08749 0.29976

#END

S127. Optimized crystal structure coordinates for first energy polymorph of **9c** for cocrystal form.

data_N2H4_BTO_2_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 17.335
_cell_length_b 6.374
_cell_length_c 8.436
_cell_angle_alpha 90.00
_cell_angle_beta 85.82
_cell_angle_gamma 90.00
_cell_volume 929.642
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
N1 N 0.51627 0.19293 0.35746
H*2 H 0.53973 0.04681 0.34299
H*3 H 0.46153 0.18735 0.32180
N4 N 0.55823 0.34692 0.26135
H*5 H 0.60045 0.40561 0.32627
H*6 H 0.58426 0.28324 0.16019
N1 N 0.74382 0.28447 0.30106
H*2 H 0.70731 0.16233 0.32904
H*3 H 0.75845 0.27844 0.18222
N4 N 0.81400 0.27016 0.38108
H*5 H 0.80499 0.34549 0.48705
H*6 H 0.82833 0.11848 0.40395
N'1+ N 0.11788 0.67682 0.22339
N'2+ N 0.20686 0.79334 0.03862
N3+ N 0.13414 0.75544 0.07984
N'4+ N 0.18559 0.66007 0.28466
C5+ C 0.23879 0.73098 0.17180
C6+ C 0.32165 0.73996 0.19035
N'7+ N 0.37490 0.81170 0.07592
N'8+ N 0.44221 0.79580 0.13540
N9+ N 0.42785 0.71684 0.28043
N'10+ N 0.35396 0.67873 0.32155
O11+ O 0.07894 0.79641 -0.02244
H*12+ H 0.03085 0.75502 0.03611
H*13+ H 0.47040 0.68810 0.35381

#END

S128. Optimized crystal structure coordinates for first energy polymorph of **9d** for cocrystal form.

data_G_BTO_2_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 23.119
_cell_length_b 13.768
_cell_length_c 4.919
_cell_angle_alpha 90.00
_cell_angle_beta 46.88
_cell_angle_gamma 90.00
_cell_volume 1142.86
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.84004 0.36079 0.26627
N'2 N 0.83314 0.27968 0.41533
H*3 H 0.80018 0.23115 0.41262
N4 N 0.87536 0.44038 0.27940
H*5 H 0.91132 0.48052 0.04298
H*6 H 0.90083 0.42215 0.37697
N7 N 0.81604 0.38153 0.07744
H*8 H 0.78105 0.33018 0.10479
H*9 H 0.79548 0.44988 0.11337
C1 C 0.11830 0.01805 -0.11039
N'2 N 0.15128 0.03988 0.01094
H*3 H 0.17343 0.10884 -0.06313
N4 N 0.09214 -0.07642 -0.07502
H*5 H 0.03964 -0.08139 -0.00550
H*6 H 0.09453 -0.11819 0.08667
N7 N 0.10340 0.08016 -0.28171
H*8 H 0.13068 0.14543 -0.35646
H*9 H 0.10865 0.04933 -0.48485
N'1+ N 0.49115 0.14860 0.26033
N'2+ N 0.53377 0.25574 0.43287
N3+ N 0.48252 0.23379 0.40841
N'4+ N 0.55377 0.10948 0.17731
C5+ C 0.57889 0.17496 0.28300
C6+ C 0.64709 0.16082 0.24132
N'7+ N 0.67202 0.22724 0.34867
N'8+ N 0.73405 0.18920 0.26766
N9+ N 0.74441 0.10306 0.11750
N'10+ N 0.69223 0.08122 0.09346
O11+ O 0.42364 0.29695 0.53165
H*12+ H 0.39443 0.26374 0.48226
H*13+ H 0.78898 0.05763 0.02831

#END

S129. Optimized crystal structure coordinates for first energy polymorph of **9e** for cocrystal form.

data_AGXR_BTO_2_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                   15.031
_cell_length_b                   9.252
_cell_length_c                   4.883
_cell_angle_alpha                90.00
_cell_angle_beta                 90.63
_cell_angle_gamma                90.00
_cell_volume                     679.022
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.35545 0.78500 0.40885
N2 N 0.36057 0.92083 0.53194
H*3 H 0.38250 0.99983 0.40535
N'4 N 0.38494 0.67325 0.54066
N5 N 0.31820 0.78405 0.14827
H*6 H 0.27047 0.85978 0.11695
H*7 H 0.29985 0.68230 0.09212
N8 N 0.36532 0.54043 0.39479
H*9 H 0.42157 0.51269 0.29119
H*10 H 0.35930 0.46360 0.54275
H*11 H 0.39586 0.91737 0.71011
C1 C 0.10006 0.62139 -0.00061
N2 N 0.05579 0.75252 -0.03800
H*3 H 0.09570 0.83393 -0.10217
N'4 N 0.08463 0.54565 0.21643
N5 N 0.15831 0.58488 -0.20715
H*6 H 0.13949 0.61955 -0.39590
H*7 H 0.17451 0.47816 -0.19838
N8 N 0.12865 0.40645 0.20597
H*9 H 0.18624 0.41568 0.31812
H*10 H 0.08962 0.33870 0.31679
H*11 H 0.02075 0.78047 0.13031
N'1+ N 0.13690 0.02961 -0.12354
N'2+ N 0.20103 0.22688 -0.29872
N3+ N 0.13122 0.14322 -0.28695
N'4+ N 0.21767 0.03710 -0.01522
C5+ C 0.25564 0.15672 -0.12281
C6+ C 0.34556 0.20575 -0.05780
N'7+ N 0.38333 0.32653 -0.16726
N'8+ N 0.46340 0.33498 -0.06129
N9+ N 0.47131 0.22175 0.10488
N'10+ N 0.40026 0.13730 0.11592
```

O11+ O 0.05708 0.17409 -0.43790
H*12+ H 0.01587 0.09667 -0.39267
H*13+ H 0.52759 0.20181 0.21469

#END

S130. Optimized crystal structure coordinates for first energy polymorph of **9f** for cocrystal form.

data_DAGXR_BTO_2_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 17.964
_cell_length_b 13.277
_cell_length_c 6.991
_cell_angle_alpha 90.00
_cell_angle_beta 116.82
_cell_angle_gamma 90.00
_cell_volume 1488.04
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C -0.13532 0.02994 -0.26996
N'2 N -0.06098 0.03069 -0.25523
N3 N -0.18127 0.11923 -0.31208
H*4 H -0.21370 0.12563 -0.22574
N5 N -0.17598 -0.05375 -0.24317
N6 N -0.14122 0.21142 -0.31123
N7 N -0.02615 -0.06931 -0.22687
H*8 H 0.00188 -0.08496 -0.06622
H*9 H -0.07913 0.20469 -0.20742
H*10 H -0.14401 0.21927 -0.45928
H*11 H 0.02133 -0.06398 -0.26779
H*12 H -0.23886 -0.05192 -0.33144
H*13 H -0.14978 -0.11866 -0.26167
C1 C 0.39075 -0.10570 0.11253
N'2 N 0.42836 -0.19168 0.16413
N3 N 0.43707 -0.01650 0.16372
H*4 H 0.41142 0.03862 0.21536
N5 N 0.30498 -0.09146 0.01021
N6 N 0.52443 -0.02180 0.29551
N7 N 0.37055 -0.27469 0.08440
H*8 H 0.34974 -0.29016 0.19553

H*9 H 0.53667 -0.08266 0.39512
H*10 H 0.55107 -0.03804 0.19774
H*11 H 0.40570 -0.33526 0.08723
H*12 H 0.28645 -0.02946 -0.08457
H*13 H 0.27496 -0.15540 -0.06592
N'1+ N 0.12710 0.06882 0.73449
N'2+ N 0.15592 0.23367 0.75640
N3+ N 0.10217 0.16265 0.73270
N'4+ N 0.20455 0.07713 0.76181
C5+ C 0.22112 0.17708 0.77478
C6+ C 0.30039 0.22000 0.80524
N'7+ N 0.31657 0.32089 0.81815
N'8+ N 0.39317 0.32998 0.84523
N9+ N 0.42021 0.23654 0.84777
N'10+ N 0.36539 0.16481 0.82366
O11+ O 0.02464 0.18623 0.70767
H*12+ H -0.00230 0.12111 0.69365
H*13+ H 0.47847 0.22152 0.86678

#END

S131. Optimized crystal structure coordinates for first energy polymorph of **9g** for cocrystal form.

data_TAGXR_BTO_2_1
_symmetry_cell_setting triclinic
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,-z
_cell_length_a 11.446
_cell_length_b 7.238
_cell_length_c 10.137
_cell_angle_alpha 91.37
_cell_angle_beta 84.64
_cell_angle_gamma 98.65
_cell_volume 826.587
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1 C 0.77524 0.49673 0.68558
N'2 N 0.70210 0.53345 0.78496
N3 N 0.64522 0.36535 0.85205
N4 N 0.80135 0.31755 0.65590
N5 N 0.85960 0.28894 0.52909
N6 N 0.83270 0.63897 0.60425
N7 N 0.83497 0.82655 0.64707
H*8 H 0.57618 0.40470 0.91095

H*9 H 0.70184 0.32747 0.91554
H*10 H 0.73149 0.21969 0.68835
H*11 H 0.91132 0.18801 0.53669
H*12 H 0.80009 0.24748 0.46145
H*13 H 0.90809 0.61254 0.55191
H*14 H 0.75427 0.86261 0.63325
H*15 H 0.83901 0.83155 0.74762
C1 C 0.72558 -0.19204 0.20535
N'2 N 0.82672 -0.22963 0.15135
N3 N 0.90019 -0.27906 0.24933
N4 N 0.69046 -0.21264 0.34025
N5 N 0.59221 -0.12646 0.39133
N6 N 0.64612 -0.13067 0.12817
N7 N 0.66136 -0.15267 -0.01093
H*8 H 0.98273 -0.27267 0.20130
H*9 H 0.87401 -0.41690 0.27268
H*10 H 0.76292 -0.19673 0.39323
H*11 H 0.54910 -0.20386 0.46826
H*12 H 0.61883 0.00618 0.42405
H*13 H 0.56057 -0.14905 0.16685
H*14 H 0.72704 -0.04946 -0.04532
H*15 H 0.69522 -0.27434 -0.03184
N'1+ N 0.08034 0.73768 0.02178
N'2+ N 0.11140 0.75665 -0.19910
N3+ N 0.03846 0.76271 -0.09261
N'4+ N 0.19141 0.71246 -0.01016
C5+ C 0.20895 0.72427 -0.14383
C6+ C 0.32044 0.70450 -0.22099
N'7+ N 0.33736 0.71661 -0.35577
N'8+ N 0.44716 0.69182 -0.38849
N9+ N 0.49206 0.66613 -0.27516
N'10+ N 0.41762 0.67244 -0.16748
O11+ O -0.07476 0.79355 -0.10185
H*12+ H -0.10944 0.79141 -0.01034
H*13+ H 0.57696 0.64343 -0.27171

#END