(Barely) Solid $Li(NH_3)_4$: The Electronics of an Expanded Metal

Eva Zurek
Department of Chemistry, State University of New York at Buffalo,
872 Natural Sciences Complex, Buffalo NY, 14260, USA

Xiao–Dong Wen and Roald Hoffmann
Department of Chemistry and Chemical Biology, Cornell University,
Baker Laboratory, Ithaca NY, 14853, USA

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1 Supporting Information

1.1 Structural Alternatives at 1 Atmosphere

The Strongly Distorted $Li(NH_3)_4$ Complex

We have performed a single–point calculation using the structural parameters found in Ref. [1] with $a = 14.8131$ Å. In this structure three of the Li–N bond lengths are short, 1.984 Å, and one is elongated, 2.488 Å. This structure was computed as being 0.298 eV per $Li(NH_3)_4$ unit higher in energy than that of the isolated molecule.

A geometry optimization was carried out starting from the experimentally determined structure in Ref. [1], keeping the lattice fixed but optimizing the position of the atoms. During the optimization the Li–N bond lengths optimized to 2.110 Å (3 bonds) and 2.112 Å (1 bond). The structure was 0.638 eV per $Li(NH_3)_4$ unit lower in energy than the isolated molecule. Thus, equalization of the Li–N bond lengths during the optimization resulted in a configuration with a much lower energy.

The aformentioned values may be compared with those of other structural alternatives in Table 1 of the main text.

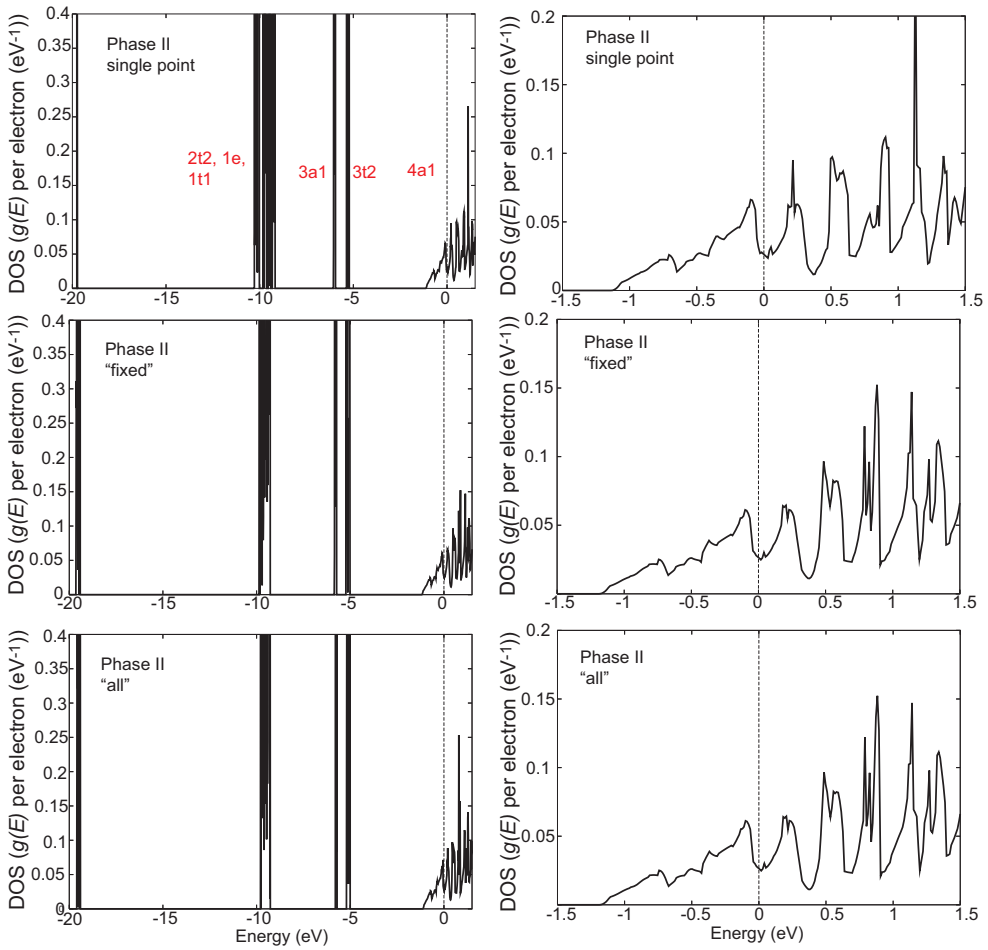

Figure S1: DOS ($g(E)$/valence electron in eV^{-1}) of the "phase II" $\mathrm{Li(NH_3)_4}$ structure, (a) a single point calculation using the structural parameters determined in Ref. [2], (b) a calculation where the lattice coordinates are kept fixed but the atomic positions are optimized, and (c) a calculation where all of the coordinates (lattice and atomic positions) are optimized. Note, the number of valence electrons per primitive cell is 264 whereas the number of excess electrons per primitive cell is 8. This is the reason why the scale on the y-axis in Fig. 4 of the main text is different.

1.2 Structural Alternatives under Pressure

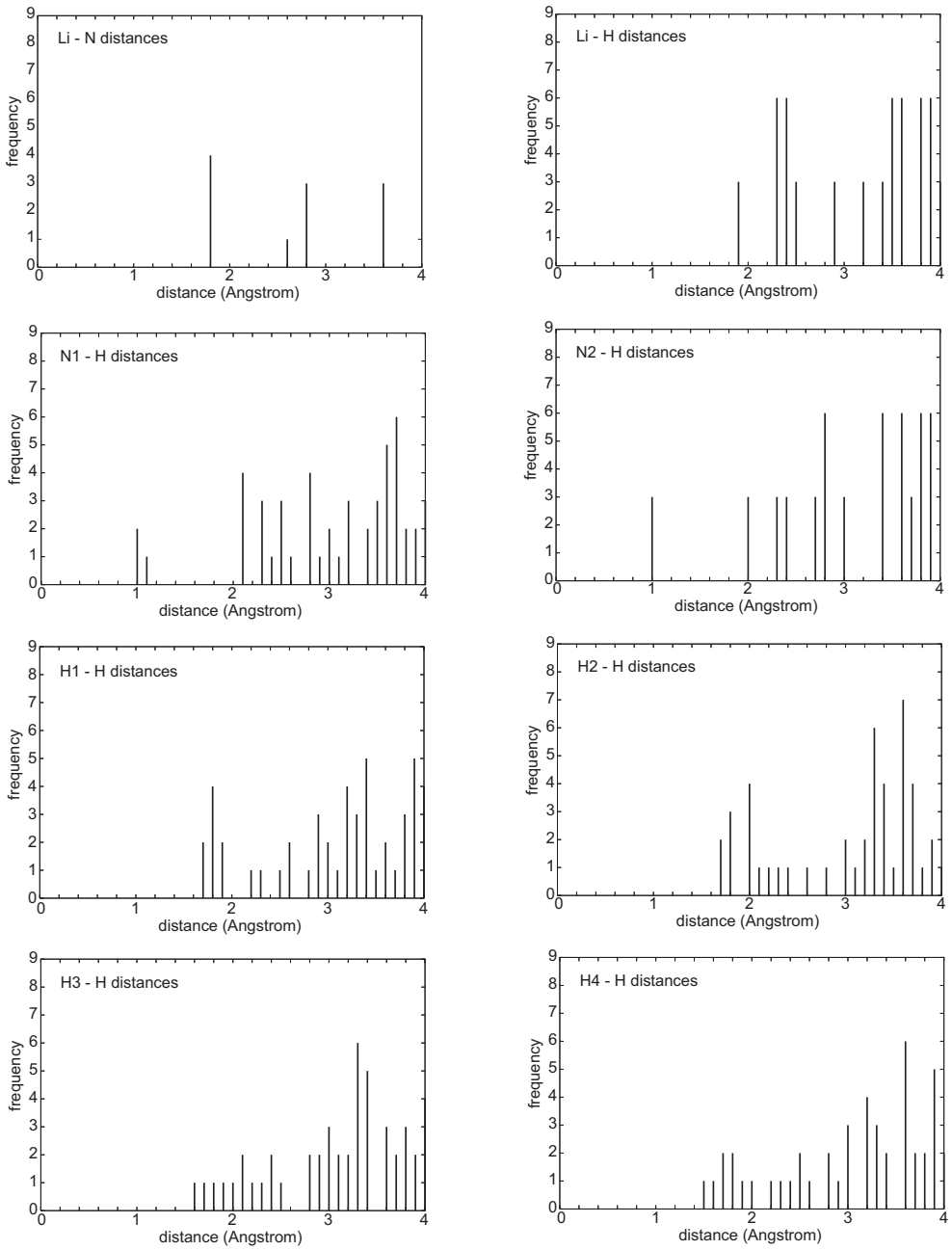

Figure S2: Histograms of Li-N, N-H, Li-H and H-H separations in "phase II" $Li(NH_3)_4$ at 50 GPa ($a = 10.282$ Å.)

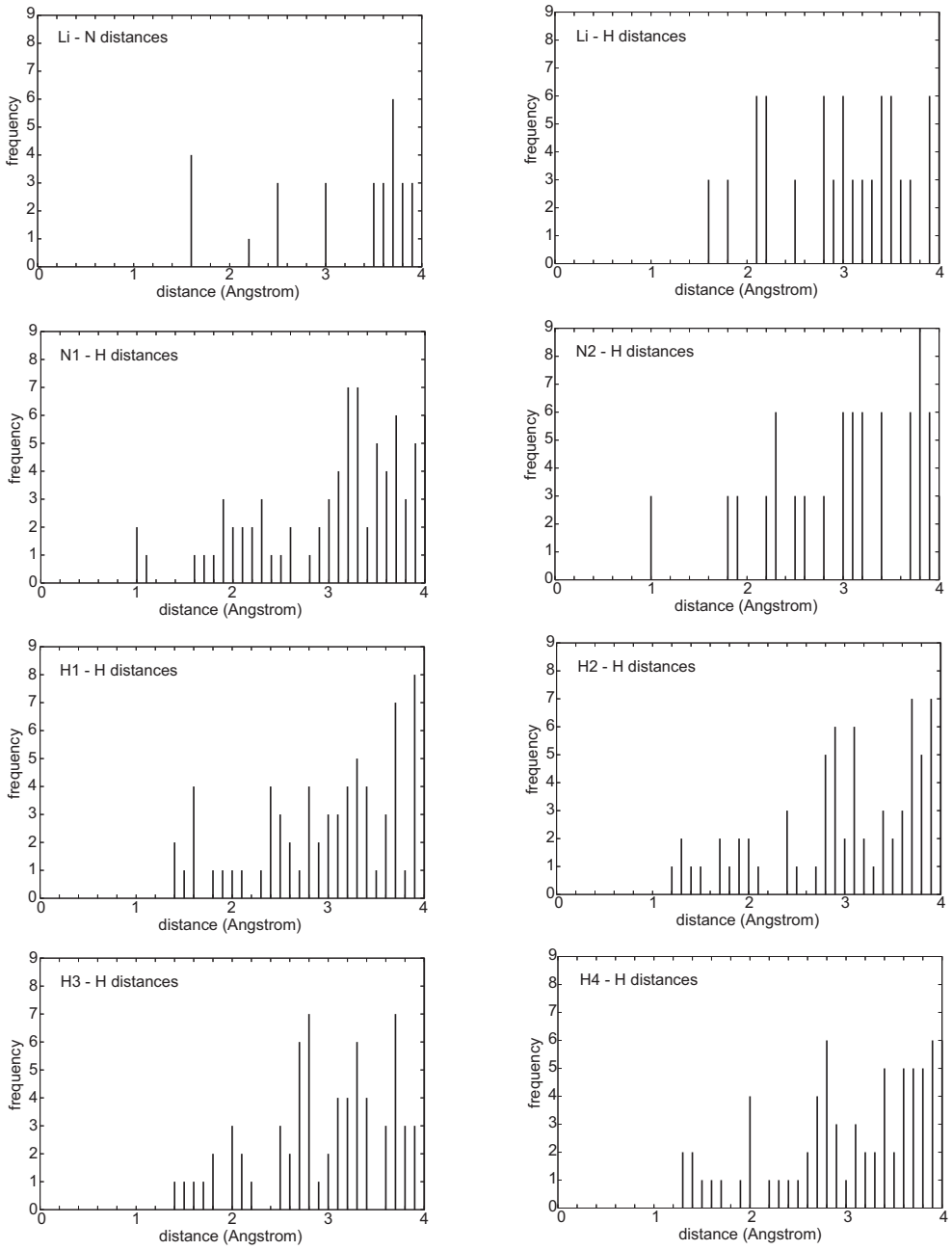

Figure S3: Histograms of Li-N, N-H, Li-H and H-H separations in "phase II" $Li(NH_3)_4$ at 200 GPa ($a = 8.890$ Å.)

1.3 Electronic Structure and Metallicity of $Li(NH_3)_4$ Under Pressure: An Unexpected Set of Bands

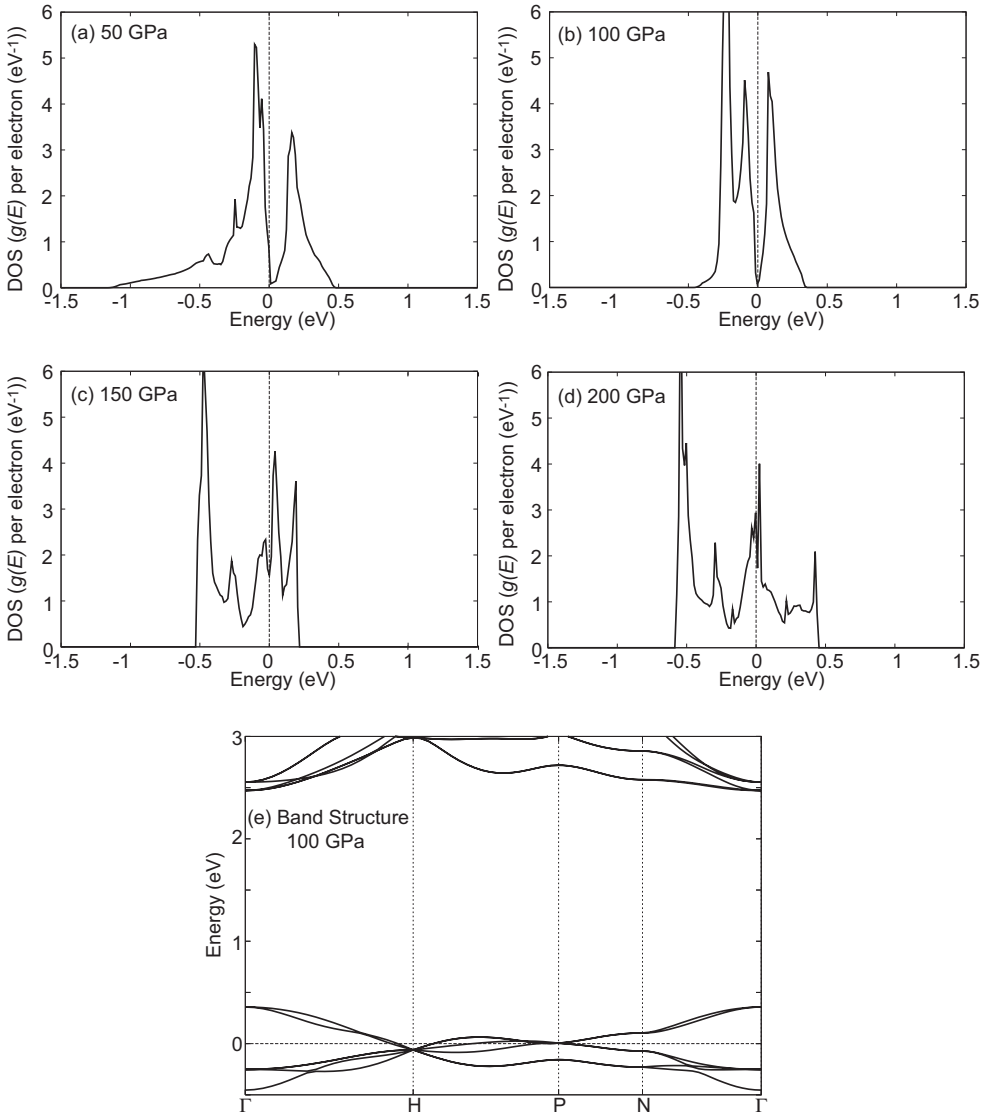

Figure S4: Valence DOS ($g(E)$/excess electron in eV^{-1}) of the optimized geometries of phase-II $Li(NH_3)_4$ at (a) 50, (b) 100, (c) 150, and (d) 200 GPa. (e) The band structure of phase II at 100 GPa. Note the four–below–two band splitting around E_F, and the large gap between these six bands, and those above.

1.4 Hydrogen–Lined Pockets in $Li(NH_3)_4$ Under Pressure

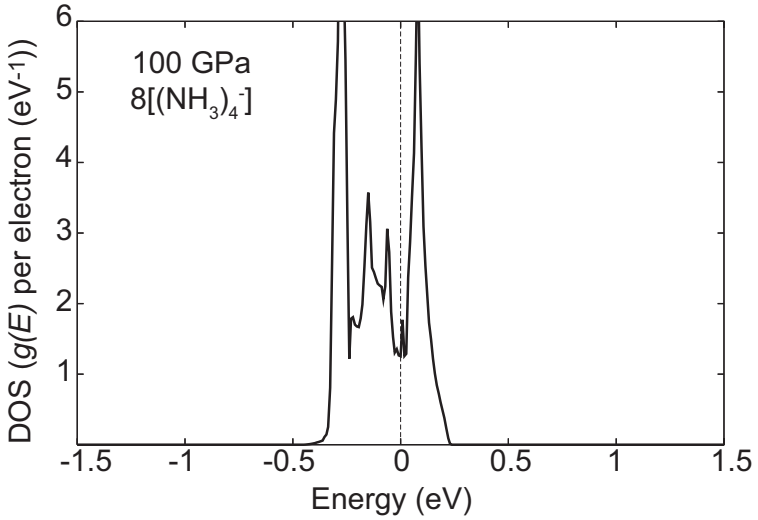

Figure S5: Valence DOS ($g(E)$/excess electron in eV^{-1}) of the "phase II" $Li(NH_3)_4$ structure, but with the Li atoms removed, and an overall charge of minus eight ($8[(NH_3)_4^-]$) at 100 GPa ($a = 9.578$ Å.)

2 Structural Parameters and Enthalpies

2.1 Simple Cubic, Space Group 215

0 GPa, Enthalpy: -81.705887 eV
$a, b, c, \alpha, \beta, \gamma$: 6.1946 6.1946 6.1946 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.29826, z = 0.11194
1 0.88806 0.70174 0.29826
8 0.11194 0.70174 0.70174
12 0.88806 0.29826 0.70174
4 0.11194 0.29826 0.29826
9 0.29826 0.88806 0.70174
2 0.70174 0.88806 0.29826
5 0.29826 0.11194 0.29826
10 0.70174 0.11194 0.70174
11 0.70174 0.29826 0.88806
6 0.29826 0.29826 0.11194
3 0.70174 0.70174 0.11194
7 0.29826 0.70174 0.88806
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000

For Nitrogen: Wyckoff position e, x = 0.19747
14 0.80253 0.80253 0.19747
16 0.19747 0.80253 0.80253
17 0.80253 0.19747 0.80253
15 0.19747 0.19747 0.19747

50 GPa, Enthalpy: -49.580915 eV
$a, b, c, \alpha, \beta, \gamma$: 4.2579 4.2579 4.2579 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.38369, z = 0.11752
1 0.88248 0.61631 0.38369
8 0.11752 0.61631 0.61631
12 0.88248 0.38369 0.61631
4 0.11752 0.38369 0.38369
9 0.38369 0.88248 0.61631
2 0.61631 0.88248 0.38369
5 0.38369 0.11752 0.38369
10 0.61631 0.11752 0.61631
11 0.61631 0.38369 0.88248
6 0.38369 0.38369 0.11752
3 0.61631 0.61631 0.11752
7 0.38369 0.61631 0.88248
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000
For Nitrogen: Wyckoff position e, x = 0.23734
14 0.76266 0.76266 0.23734
16 0.23734 0.76266 0.76266
17 0.76266 0.23734 0.76266
15 0.23734 0.23734 0.23734

100 GPa, Enthalpy: -28.032137 eV
$a, b, c, \alpha, \beta, \gamma$: 3.9731 3.9731 3.9731 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.39134, z = 0.11465
1 0.88535 0.60866 0.39134
8 0.11465 0.60866 0.60866
12 0.88535 0.39134 0.60866
4 0.11465 0.39134 0.39134
9 0.39134 0.88535 0.60866
2 0.60866 0.88535 0.39134
5 0.39134 0.11465 0.39134
10 0.60866 0.11465 0.60866
11 0.60866 0.39134 0.88535
6 0.39134 0.39134 0.11465
3 0.60866 0.60866 0.11465

7 0.39134 0.60866 0.88535
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000
For Nitrogen: Wyckoff position e, x = 0.23608
14 0.76392 0.76392 0.23608
16 0.23608 0.76392 0.76392
17 0.76392 0.23608 0.76392
15 0.23608 0.23608 0.23608

150 GPa, Enthalpy: -9.728215 eV
$a, b, c, \alpha, \beta, \gamma$: 3.9731 3.9731 3.9731 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.39134, z = 0.11465
1 0.88535 0.60866 0.39134
8 0.11465 0.60866 0.60866
12 0.88535 0.39134 0.60866
4 0.11465 0.39134 0.39134
9 0.39134 0.88535 0.60866
2 0.60866 0.88535 0.39134
5 0.39134 0.11465 0.39134
10 0.60866 0.11465 0.60866
11 0.60866 0.39134 0.88535
6 0.39134 0.39134 0.11465
3 0.60866 0.60866 0.11465
7 0.39134 0.60866 0.88535
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000
For Nitrogen: Wyckoff position e, x = 0.23608
14 0.76392 0.76392 0.23608
16 0.23608 0.76392 0.76392
17 0.76392 0.23608 0.76392
15 0.23608 0.23608 0.23608

200 GPa, Enthalpy: 6.651799 eV
$a, b, c, \alpha, \beta, \gamma$: 3.6864 3.6864 3.6864 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.39849, z = 0.11474
1 0.88526 0.60151 0.39849
8 0.11474 0.60151 0.60151
12 0.88526 0.39849 0.60151
4 0.11474 0.39849 0.39849
9 0.39849 0.88526 0.60151
2 0.60151 0.88526 0.39849
5 0.39849 0.11474 0.39849
10 0.60151 0.11474 0.60151

11 0.60151 0.39849 0.88526
6 0.39849 0.39849 0.11474
3 0.60151 0.60151 0.11474
7 0.39849 0.60151 0.88526
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000
For Nitrogen: Wyckoff position e, x = 0.23429
14 0.76571 0.76571 0.23429
16 0.23429 0.76571 0.76571
17 0.76571 0.23429 0.76571
15 0.23429 0.23429 0.23429

2.2 Body Centered Cubic (Conventional Cell), Space Group 215

0 GPa, Enthalpy: -163.490658 eV
$a, b, c, \alpha, \beta, \gamma$: 7.8724 7.8724 7.8724 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.23317, z = 0.08597
1 0.91403 0.76683 0.23317
8 0.08597 0.76683 0.76683
12 0.91403 0.23317 0.76683
4 0.08597 0.23317 0.23317
9 0.23317 0.91403 0.76683
2 0.76683 0.91403 0.23317
5 0.23317 0.08597 0.23317
10 0.76683 0.08597 0.76683
11 0.76683 0.23317 0.91403
6 0.23317 0.23317 0.08597
3 0.76683 0.76683 0.08597
7 0.23317 0.76683 0.91403
For Hydrogen: Wyckoff position i, x = 0.26683, z = -0.41404
13 0.41404 0.26683 0.73317
20 0.58596 0.26683 0.26683
24 0.41404 0.73317 0.26683
16 0.58596 0.73317 0.73317
21 0.73317 0.41404 0.26683
14 0.26683 0.41404 0.73317
17 0.73317 0.58596 0.73317
22 0.26683 0.58596 0.26683
23 0.26683 0.73317 0.41404
18 0.73317 0.73317 0.58596
15 0.26683 0.26683 0.58596
19 0.73317 0.26683 0.41404
For Lithium: Wyckoff position a

25 0.00000 0.00000 0.00000
For Lithium: Wyckoff position b
26 0.50000 0.50000 0.50000
For Nitrogen: Wyckoff position e, x = 0.15448
27 0.84552 0.84552 0.15448
29 0.15448 0.84552 0.84552
30 0.84552 0.15448 0.84552
28 0.15448 0.15448 0.15448
For Nitrogen: Wyckoff position e, x = -0.34552
31 0.34552 0.34552 0.65448
33 0.65448 0.34552 0.34552
34 0.34552 0.65448 0.34552
32 0.65448 0.65448 0.65448

50 GPa, Enthalpy: -104.747266 eV
$a, b, c, \alpha, \beta, \gamma$: 5.1239 5.1239 5.1239 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.35087, z = 0.13379
1 0.86621 0.64913 0.35087
8 0.13379 0.64913 0.64913
12 0.86621 0.35087 0.64913
4 0.13379 0.35087 0.35087
9 0.35087 0.86621 0.64913
2 0.64913 0.86621 0.35087
5 0.35087 0.13379 0.35087
10 0.64913 0.13379 0.64913
11 0.64913 0.35087 0.86621
6 0.35087 0.35087 0.13379
3 0.64913 0.64913 0.13379
7 0.35087 0.64913 0.86621
For Hydrogen: Wyckoff position i, x = 0.14913, z = -0.36621
13 0.36621 0.14913 0.85087
20 0.63379 0.14913 0.14913
24 0.36621 0.85087 0.14913
16 0.63379 0.85087 0.85087
21 0.85087 0.36621 0.14913
14 0.14913 0.36621 0.85087
17 0.85087 0.63379 0.85087
22 0.14913 0.63379 0.14913
23 0.14913 0.85087 0.36621
18 0.85087 0.85087 0.63379
15 0.14913 0.14913 0.63379
19 0.85087 0.14913 0.36621
For Lithium: Wyckoff position a

25 0.00000 0.00000 0.00000
For Lithium Wyckoff position b
26 0.50000 0.50000 0.50000
For Nitrogen: Wyckoff position e, x = 0.22349
27 0.77651 0.77651 0.22349
29 0.22349 0.77651 0.77651
30 0.77651 0.22349 0.77651
28 0.22349 0.22349 0.22349
For Nitrogen: Wyckoff position e, x = -0.27651
31 0.27651 0.27651 0.72349
33 0.72349 0.27651 0.27651
34 0.27651 0.72349 0.27651
32 0.72349 0.72349 0.72349

100 GPa, Enthalpy: -66.870015 eV
$a, b, c, \alpha, \beta, \gamma$: 4.8070 4.8070 4.8070 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.36087, z = 0.13334
1 0.86666 0.63913 0.36087
8 0.13334 0.63913 0.63913
12 0.86666 0.36087 0.63913
4 0.13334 0.36087 0.36087
9 0.36087 0.86666 0.63913
2 0.63913 0.86666 0.36087
5 0.36087 0.13334 0.36087
10 0.63913 0.13334 0.63913
11 0.63913 0.36087 0.86666
6 0.36087 0.36087 0.13334
3 0.63913 0.63913 0.13334
7 0.36087 0.63913 0.86666
For Hydrogen: Wyckoff position i, x = 0.13913, z = -0.36666
13 0.36666 0.13913 0.86087
20 0.63334 0.13913 0.13913
24 0.36666 0.86087 0.13913
16 0.63334 0.86087 0.86087
21 0.86087 0.36666 0.13913
14 0.13913 0.36666 0.86087
17 0.86087 0.63334 0.86087
22 0.13913 0.63334 0.13913
23 0.13913 0.86087 0.36666
18 0.86087 0.86087 0.63334
15 0.13913 0.13913 0.63334
19 0.86087 0.13913 0.36666
For Lithium: Wyckoff position a

25 0.00000 0.00000 0.00000
For Lithium: Wyckoff position b
26 0.50000 0.50000 0.50000
For Nitrogen: Wyckoff position e, x = 0.22547
27 0.77453 0.77453 0.22547
29 0.22547 0.77453 0.77453
30 0.77453 0.22547 0.77453
28 0.22547 0.22547 0.22547
For Nitrogen: Wyckoff position e, x = -0.27453
31 0.27453 0.27453 0.72547
33 0.72547 0.27453 0.27453
34 0.27453 0.72547 0.27453
32 0.72547 0.72547 0.72547

150 GPa, Enthalpy: -34.285404 eV
$a, b, c, \alpha, \beta, \gamma$: 4.6185 4.6185 4.6185 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.36608, z = 0.13213
1 0.86787 0.63392 0.36608
8 0.13213 0.63392 0.63392
12 0.86787 0.36608 0.63392
4 0.13213 0.36608 0.36608
9 0.36608 0.86787 0.63392
2 0.63392 0.86787 0.36608
5 0.36608 0.13213 0.36608
10 0.63392 0.13213 0.63392
11 0.63392 0.36608 0.86787
6 0.36608 0.36608 0.13213
3 0.63392 0.63392 0.13213
7 0.36608 0.63392 0.86787
For Hydrogen: Wyckoff position i, x = 0.13392, z = -0.36787
13 0.36787 0.13392 0.86608
20 0.63213 0.13392 0.13392
24 0.36787 0.86608 0.13392
16 0.63213 0.86608 0.86608
21 0.86608 0.36787 0.13392
14 0.13392 0.36787 0.86608
17 0.86608 0.63213 0.86608
22 0.13392 0.63213 0.13392
23 0.13392 0.86608 0.36787
18 0.86608 0.86608 0.63213
15 0.13392 0.13392 0.63213
19 0.86608 0.13392 0.36787
For Lithium: Wyckoff position a

25 0.00000 0.00000 0.00000
For Lithium: Wyckoff position b
26 0.50000 0.50000 0.50000
For Nitrogen: Wyckoff position e, x = 0.22582
27 0.77418 0.77418 0.22582
29 0.22582 0.77418 0.77418
30 0.77418 0.22582 0.77418
28 0.22582 0.22582 0.22582
For Nitrogen: Wyckoff position e, x = -0.27418
31 0.27418 0.27418 0.72582
33 0.72582 0.27418 0.27418
34 0.27418 0.72582 0.27418
32 0.72582 0.72582 0.72582

200 GPa, Enthalpy: -4.905146 eV
$a, b, c, \alpha, \beta, \gamma$: 4.4824 4.4824 4.4824 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.37029, z = 0.13152
1 0.86848 0.62971 0.37029
8 0.13152 0.62971 0.62971
12 0.86848 0.37029 0.62971
4 0.13152 0.37029 0.37029
9 0.37029 0.86848 0.62971
2 0.62971 0.86848 0.37029
5 0.37029 0.13152 0.37029
10 0.62971 0.13152 0.62971
11 0.62971 0.37029 0.86848
6 0.37029 0.37029 0.13152
3 0.62971 0.62971 0.13152
7 0.37029 0.62971 0.86848
For Hydrogen: Wyckoff position i, x = 0.12971, z = -0.36848
13 0.36848 0.12971 0.87029
20 0.63152 0.12971 0.12971
24 0.36848 0.87029 0.12971
16 0.63152 0.87029 0.87029
21 0.87029 0.36848 0.12971
14 0.12971 0.36848 0.87029
17 0.87029 0.63152 0.87029
22 0.12971 0.63152 0.12971
23 0.12971 0.87029 0.36848
18 0.87029 0.87029 0.63152
15 0.12971 0.12971 0.63152
19 0.87029 0.12971 0.36848
For Lithium: Wyckoff position a

25 0.00000 0.00000 0.00000
For Lithium: Wyckoff position b
26 0.50000 0.50000 0.50000
For Nitrogen: Wyckoff position e, x = 0.22654
27 0.77346 0.77346 0.22654
29 0.22654 0.77346 0.77346
30 0.77346 0.22654 0.77346
28 0.22654 0.22654 0.22654
For Nitrogen: Wyckoff position e, x = -0.27346
31 0.27346 0.27346 0.72654
33 0.72654 0.27346 0.27346
34 0.27346 0.72654 0.27346
32 0.72654 0.72654 0.72654

2.3 Face Centered Cubic, Space Group 216

0 GPa, Enthalpy: -81.587331 eV
$a, b, c, \alpha, \beta, \gamma$: 10.94936 10.94936 10.94936 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position h, x = 0.33360, z = -0.06047
1 0.83360 0.93953 0.83360
12 0.66640 0.93953 0.66640
8 0.83360 0.56047 0.66640
4 0.66640 0.56047 0.83360
3 0.83360 0.83360 0.93953
11 0.66640 0.83360 0.56047
7 0.83360 0.66640 0.56047
6 0.66640 0.66640 0.93953
2 0.93953 0.83360 0.83360
10 0.56047 0.83360 0.66640
9 0.93953 0.66640 0.66640
5 0.56047 0.66640 0.83360
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000
For Nitrogen: Wyckoff position e, x = -0.11000
14 0.89000 0.89000 0.89000
17 0.61000 0.89000 0.61000
16 0.89000 0.61000 0.61000
15 0.61000 0.61000 0.89000

50 GPa, Enthalpy: -39.702067 eV
$a, b, c, \alpha, \beta, \gamma$: 7.16195 7.16195 7.16195 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position h, x = 0.32437, z = -0.00544

1 0.82437 0.99456 0.82437
12 0.67563 0.99456 0.67563
8 0.82437 0.50544 0.67563
4 0.67563 0.50544 0.82437
3 0.82437 0.82437 0.99456
11 0.67563 0.82437 0.50544
7 0.82437 0.67563 0.50544
6 0.67563 0.67563 0.99456
2 0.99456 0.82437 0.82437
10 0.50544 0.82437 0.67563
9 0.99456 0.67563 0.67563
5 0.50544 0.67563 0.82437
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000
For Nitrogen: Wyckoff position e, x = -0.13224
14 0.86776 0.86776 0.86776
17 0.63224 0.86776 0.63224
16 0.86776 0.63224 0.63224
15 0.63224 0.63224 0.86776

100 GPa, Enthalpy: -14.607249 eV
$a, b, c, \alpha, \beta, \gamma$: 6.58593 6.58593 6.58593 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position h, x = 0.32519, z = 0.00834
1 0.32519 0.00834 0.32519
12 0.17481 0.00834 0.17481
8 0.32519 0.49166 0.17481
4 0.17481 0.49166 0.32519
3 0.32519 0.32519 0.00834
11 0.17481 0.32519 0.49166
7 0.32519 0.17481 0.49166
6 0.17481 0.17481 0.00834
2 0.00834 0.32519 0.32519
10 0.49166 0.32519 0.17481
9 0.00834 0.17481 0.17481
5 0.49166 0.17481 0.32519
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000
For Nitrogen: Wyckoff position e, x = -0.13609
14 0.86391 0.86391 0.86391
17 0.63609 0.86391 0.63609
16 0.86391 0.63609 0.63609
15 0.63609 0.63609 0.86391

150 GPa, Enthalpy: 5.666152 eV

$a, b, c, \alpha, \beta, \gamma$: 6.19151 6.19151 6.19151 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position h, x = 0.32321, z = 0.02112
1 0.32321 0.02112 0.32321
12 0.17679 0.02112 0.17679
8 0.32321 0.47888 0.17679
4 0.17679 0.47888 0.32321
3 0.32321 0.32321 0.02112
11 0.17679 0.32321 0.47888
7 0.32321 0.17679 0.47888
6 0.17679 0.17679 0.02112
2 0.02112 0.32321 0.32321
10 0.47888 0.32321 0.17679
9 0.02112 0.17679 0.17679
5 0.47888 0.17679 0.32321
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000
For Nitrogen: Wyckoff position e, x = -0.14023
14 0.85977 0.85977 0.85977
17 0.64023 0.85977 0.64023
16 0.85977 0.64023 0.64023
15 0.64023 0.64023 0.85977

200 GPa, Enthalpy: 22.774791 eV
$a, b, c, \alpha, \beta, \gamma$: 5.86096 5.86096 5.86096 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position h, x = 0.31840, z = 0.04121
1 0.31840 0.04121 0.31840
12 0.18160 0.04121 0.18160
8 0.31840 0.45879 0.18160
4 0.18160 0.45879 0.31840
3 0.31840 0.31840 0.04121
11 0.18160 0.31840 0.45879
7 0.31840 0.18160 0.45879
6 0.18160 0.18160 0.04121
2 0.04121 0.31840 0.31840
10 0.45879 0.31840 0.18160
9 0.04121 0.18160 0.18160
5 0.45879 0.18160 0.31840
For Lithium: Wyckoff position a
13 0.00000 0.00000 0.00000
For Nitrogen: Wyckoff position e, x = -0.14701
14 0.85299 0.85299 0.85299
17 0.64701 0.85299 0.64701

16 0.85299 0.64701 0.64701
15 0.64701 0.64701 0.85299

2.4 Cs-IV, Space Group 141

0 GPa, Enthalpy: -163.490920 eV
$a, b, c, \alpha, \beta, \gamma$: 10.12397 10.12397 8.83603 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = 0.23048, y = 0.33061, z
1 0.23048 0.33061 0.00320
6 0.23048 0.66939 0.99680
5 0.26952 0.33061 0.49680
2 0.76952 0.16939 0.00320
8 0.41939 0.51952 0.24680
3 0.41939 0.48048 0.75320
4 0.08061 0.51952 0.25320
7 0.58061 0.98048 0.24680
9 0.26952 0.16939 0.49680
14 0.76952 0.33061 0.00320
13 0.23048 0.16939 0.00320
10 0.23048 0.83061 0.99680
16 0.58061 0.48048 0.75320
11 0.58061 0.51952 0.24680
12 0.41939 0.98048 0.24680
15 0.91939 0.51952 0.25320
For Hydrogen: Wyckoff position h, y = 0.10459, z = -0.37982
17 0.14541 0.25000 0.12982
22 0.14541 0.75000 0.87018
21 0.35459 0.25000 0.37018
18 0.35459 0.75000 0.62982
24 0.50000 0.60459 0.12018
19 0.50000 0.39541 0.87982
20 0.00000 0.60459 0.37982
23 0.00000 0.39541 0.62018
For Lithium: Wyckoff position a
25 0.00000 0.25000 0.87500
26 0.00000 0.75000 0.12500
For Nitrogen: Wyckoff position h, y = 0.08038, z = -0.26663
27 0.16962 0.25000 0.01663
32 0.16962 0.75000 0.98337
31 0.33038 0.25000 0.48337
28 0.83038 0.25000 0.01663
34 0.50000 0.58038 0.23337
29 0.50000 0.41962 0.76663

30 0.00000 0.58038 0.26663
33 0.50000 0.91962 0.23337
50 GPa, Enthalpy: -102.055869 eV
$a, b, c, \alpha, \beta, \gamma$: 7.13071 7.13071 5.28978 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.23038, y = -0.12175, z
1 0.26962 0.37825 0.91805
7 0.12825 0.51962 0.83195
8 0.37175 0.48038 0.33195
2 0.23038 0.62175 0.41805
6 0.26962 0.62175 0.08195
3 0.37175 0.51962 0.66805
4 0.12825 0.48038 0.16805
5 0.23038 0.37825 0.58195
9 0.23038 0.12175 0.58195
15 0.87175 0.48038 0.16805
16 0.62825 0.51962 0.66805
10 0.26962 0.87825 0.08195
14 0.73038 0.37825 0.91805
11 0.12825 0.98038 0.83195
12 0.37175 0.01962 0.33195
13 0.76962 0.62175 0.41805
For Hydrogen: Wyckoff position h, y = 0.07999, z = -0.40924
17 0.17001 0.25000 0.15924
23 0.00000 0.42001 0.59076
24 0.50000 0.57999 0.09076
18 0.32999 0.75000 0.65924
22 0.17001 0.75000 0.84076
19 0.50000 0.42001 0.90924
20 0.00000 0.57999 0.40924
21 0.32999 0.25000 0.34076
For Lithium: Wyckoff position a
25 0.00000 0.25000 0.87500
26 0.00000 0.75000 0.12500
For Nitrogen: Wyckoff position h, y = -0.00316, z = -0.25275
27 0.25316 0.25000 0.00275
33 0.50000 0.00316 0.24725
34 0.50000 0.49684 0.24725
28 0.74684 0.25000 0.00275
32 0.25316 0.75000 0.99725
29 0.50000 0.50316 0.75275
30 0.00000 0.49684 0.25275
31 0.24684 0.25000 0.49725

100 GPa, Enthalpy: -64.533506 eV
$a, b, c, \alpha, \beta, \gamma$: 6.61628 6.61628 4.98813 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.22856, y = -0.11429, z
1 0.27144 0.38571 0.90716
7 0.13571 0.52144 0.84284
8 0.36429 0.47856 0.34284
2 0.22856 0.61429 0.40716
6 0.27144 0.61429 0.09284
3 0.36429 0.52144 0.65716
4 0.13571 0.47856 0.15716
5 0.22856 0.38571 0.59284
9 0.22856 0.11429 0.59284
15 0.86429 0.47856 0.15716
16 0.63571 0.52144 0.65716
10 0.27144 0.88571 0.09284
14 0.72856 0.38571 0.90716
11 0.13571 0.97856 0.84284
12 0.36429 0.02144 0.34284
13 0.77144 0.61429 0.40716
For Hydrogen: Wyckoff position h, y = 0.08409, z = -0.40863
17 0.16591 0.25000 0.15863
23 0.00000 0.41591 0.59137
24 0.50000 0.58409 0.09137
18 0.33409 0.75000 0.65863
22 0.16591 0.75000 0.84137
19 0.50000 0.41591 0.90863
20 0.00000 0.58409 0.40863
21 0.33409 0.25000 0.34137
For Lithium: Wyckoff position a
25 0.00000 0.25000 0.87500
26 0.00000 0.75000 0.12500
For Nitrogen: Wyckoff position h, y = -0.01427, z = -0.25134
27 0.26427 0.25000 0.00134
33 0.50000 0.01427 0.24866
34 0.50000 0.48573 0.24866
28 0.73573 0.25000 0.00134
32 0.26427 0.75000 0.99866
29 0.50000 0.51427 0.75134
30 0.00000 0.48573 0.25134
31 0.23573 0.25000 0.49866

150 GPa, Enthalpy: -32.632234 eV
$a, b, c, \alpha, \beta, \gamma$: 6.32213 6.32213 4.80689 90.00000 90.00000 90.00000

Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.22618, y = -0.10969, z
1 0.27382 0.39031 0.90242
7 0.14031 0.52382 0.84758
8 0.35969 0.47618 0.34758
2 0.22618 0.60969 0.40242
6 0.27382 0.60969 0.09758
3 0.35969 0.52382 0.65242
4 0.14031 0.47618 0.15242
5 0.22618 0.39031 0.59758
9 0.22618 0.10969 0.59758
15 0.85969 0.47618 0.15242
16 0.64031 0.52382 0.65242
10 0.27382 0.89031 0.09758
14 0.72618 0.39031 0.90242
11 0.14031 0.97618 0.84758
12 0.35969 0.02382 0.34758
13 0.77382 0.60969 0.40242
For Hydrogen: Wyckoff position h, y = 0.08719, z = -0.40980
17 0.16281 0.25000 0.15980
23 0.00000 0.41281 0.59020
24 0.50000 0.58719 0.09020
18 0.33719 0.75000 0.65980
22 0.16281 0.75000 0.84020
19 0.50000 0.41281 0.90980
20 0.00000 0.58719 0.40980
21 0.33719 0.25000 0.34020
For Lithium: Wyckoff position a
25 0.00000 0.25000 0.87500
26 0.00000 0.75000 0.12500
For Nitrogen: Wyckoff position h, y = -0.01882, z = -0.25008
27 0.26882 0.25000 0.00008
33 0.50000 0.01882 0.24992
34 0.50000 0.48118 0.24992
28 0.73118 0.25000 0.00008
32 0.26882 0.75000 0.99992
29 0.50000 0.51882 0.75008
30 0.00000 0.48118 0.25008
31 0.23118 0.25000 0.49992

200 GPa, Enthalpy: -4.064378 eV
$a, b, c, \alpha, \beta, \gamma$: 6.11444 6.11444 4.67448 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position i, x = -0.22443, y = -0.10648, z

1 0.27557 0.39352 0.89820
7 0.14352 0.52557 0.85180
8 0.35648 0.47443 0.35180
2 0.22443 0.60648 0.39820
6 0.27557 0.60648 0.10180
3 0.35648 0.52557 0.64820
4 0.14352 0.47443 0.14820
5 0.22443 0.39352 0.60180
9 0.22443 0.10648 0.60180
15 0.85648 0.47443 0.14820
16 0.64352 0.52557 0.64820
10 0.27557 0.89352 0.10180
14 0.72443 0.39352 0.89820
11 0.14352 0.97443 0.85180
12 0.35648 0.02557 0.35180
13 0.77557 0.60648 0.39820
For Hydrogen: Wyckoff position h, y = 0.08892, z = -0.41045
17 0.16108 0.25000 0.16045
23 0.00000 0.41108 0.58955
24 0.50000 0.58892 0.08955
18 0.33892 0.75000 0.66045
22 0.16108 0.75000 0.83955
19 0.50000 0.41108 0.91045
20 0.00000 0.58892 0.41045
21 0.33892 0.25000 0.33955
For Lithium: Wyckoff position a
25 0.00000 0.25000 0.87500
26 0.00000 0.75000 0.12500
For Nitrogen: Wyckoff position h, y = -0.02275, z = -0.24857
27 0.27275 0.25000 0.99857
33 0.50000 0.02275 0.25143
34 0.50000 0.47725 0.25143
28 0.72725 0.25000 0.99857
32 0.27275 0.75000 0.00143
29 0.50000 0.52275 0.74857
30 0.00000 0.47725 0.24857
31 0.22725 0.25000 0.50143

2.5 $P2_13$, Space Group 198

0 GPa, Enthalpy: -326.746261 eV
$a, b, c, \alpha, \beta, \gamma$: 9.90217 9.90217 9.90217 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:

For Hydrogen: Wyckoff position b, x = 0.19749, y = -0.48189, z
1 0.19749 0.51811 0.50323
13 0.30251 0.48189 0.00323
9 0.80251 0.01811 0.99677
5 0.69749 0.98189 0.49677
45 0.50323 0.19749 0.51811
37 0.99677 0.80251 0.01811
41 0.49677 0.69749 0.98189
33 0.00323 0.30251 0.48189
21 0.51811 0.50323 0.19749
17 0.98189 0.49677 0.69749
25 0.48189 0.00323 0.30251
29 0.01811 0.99677 0.80251
For Hydrogen: Wyckoff position b, x = 0.32625, y = -0.40130, z
2 0.32625 0.59870 0.43882
14 0.17375 0.40130 0.93882
10 0.67375 0.09870 0.06118
6 0.82625 0.90130 0.56118
46 0.43882 0.32625 0.59870
38 0.06118 0.67375 0.09870
42 0.56118 0.82625 0.90130
34 0.93882 0.17375 0.40130
22 0.59870 0.43882 0.32625
18 0.90130 0.56118 0.82625
26 0.40130 0.93882 0.17375
30 0.09870 0.06118 0.67375
For Hydrogen: Wyckoff position b, x = 0.18941, y = -0.42424, z
3 0.18941 0.57576 0.34907
15 0.31059 0.42424 0.84907
11 0.81059 0.07576 0.15093
7 0.68941 0.92424 0.65093
47 0.34907 0.18941 0.57576
39 0.15093 0.81059 0.07576
43 0.65093 0.68941 0.92424
35 0.84907 0.31059 0.42424
23 0.57576 0.34907 0.18941
19 0.92424 0.65093 0.68941
27 0.42424 0.84907 0.31059
31 0.07576 0.15093 0.81059
For Hydrogen: Wyckoff position b, x = 0.20084, y = 0.13589, z
4 0.20084 0.13589 0.27055
16 0.29916 0.86411 0.77055
12 0.79916 0.63589 0.22945
8 0.70084 0.36411 0.72945

48 0.27055 0.20084 0.13589
40 0.22945 0.79916 0.63589
44 0.72945 0.70084 0.36411
36 0.77055 0.29916 0.86411
24 0.13589 0.27055 0.20084
20 0.36411 0.72945 0.70084
28 0.86411 0.77055 0.29916
32 0.63589 0.22945 0.79916
For Lithium: Wyckoff position a, x = 0.34971
49 0.34971 0.34971 0.34971
52 0.15029 0.65029 0.84971
51 0.65029 0.84971 0.15029
50 0.84971 0.15029 0.65029
For Nitrogen: Wyckoff position b, x = 0.25308, y = -0.47166, z
53 0.25308 0.52834 0.41613
56 0.24692 0.47166 0.91613
55 0.74692 0.02834 0.08387
54 0.75308 0.97166 0.58387
64 0.41613 0.25308 0.52834
62 0.08387 0.74692 0.02834
63 0.58387 0.75308 0.97166
61 0.91613 0.24692 0.47166
58 0.52834 0.41613 0.25308
57 0.97166 0.58387 0.75308
59 0.47166 0.91613 0.24692
60 0.02834 0.08387 0.74692
For Nitrogen: Wyckoff position a, x = 0.22651
65 0.22651 0.22651 0.22651
68 0.27349 0.77349 0.72651
67 0.77349 0.72651 0.27349
66 0.72651 0.27349 0.77349

50 GPa, Enthalpy: -209.449891 eV
$a, b, c, \alpha, \beta, \gamma$: 6.52954 6.52954 6.52954 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position b, x = -0.36645, y = 0.09738, z
1 0.63355 0.09738 0.03345
13 0.86645 0.90262 0.53345
9 0.36645 0.59738 0.46655
5 0.13355 0.40262 0.96655
45 0.03345 0.63355 0.09738
37 0.46655 0.36645 0.59738
41 0.96655 0.13355 0.40262
33 0.53345 0.86645 0.90262

21 0.09738 0.03345 0.63355
17 0.40262 0.96655 0.13355
25 0.90262 0.53345 0.86645
29 0.59738 0.46655 0.36645
For Hydrogen: Wyckoff position b, x = -0.12525, y = 0.07645, z
2 0.87475 0.07645 0.96101
14 0.62525 0.92355 0.46101
10 0.12525 0.57645 0.53899
6 0.37475 0.42355 0.03899
46 0.96101 0.87475 0.07645
38 0.53899 0.12525 0.57645
42 0.03899 0.37475 0.42355
34 0.46101 0.62525 0.92355
22 0.07645 0.96101 0.87475
18 0.42355 0.03899 0.37475
26 0.92355 0.46101 0.62525
30 0.57645 0.53899 0.12525
For Hydrogen: Wyckoff position b, x = -0.31542, y = 0.13538, z
3 0.68458 0.13538 0.79007
15 0.81542 0.86462 0.29007
11 0.31542 0.63538 0.70993
7 0.18458 0.36462 0.20993
47 0.79007 0.68458 0.13538
39 0.70993 0.31542 0.63538
43 0.20993 0.18458 0.36462
35 0.29007 0.81542 0.86462
23 0.13538 0.79007 0.68458
19 0.36462 0.20993 0.18458
27 0.86462 0.29007 0.81542
31 0.63538 0.70993 0.31542
For Hydrogen: Wyckoff position b, x = -0.39000, y = -0.45659, z
4 0.61000 0.54341 0.75691
16 0.89000 0.45659 0.25691
12 0.39000 0.04341 0.74309
8 0.11000 0.95659 0.24309
48 0.75691 0.61000 0.54341
40 0.74309 0.39000 0.04341
44 0.24309 0.11000 0.95659
36 0.25691 0.89000 0.45659
24 0.54341 0.75691 0.61000
20 0.95659 0.24309 0.11000
28 0.45659 0.25691 0.89000
32 0.04341 0.74309 0.39000
For Lithium: Wyckoff position a, x = -0.18676

49 0.81324 0.81324 0.81324
52 0.68676 0.18676 0.31324
51 0.18676 0.31324 0.68676
50 0.31324 0.68676 0.18676
For Nitrogen: Wyckoff position b, x = -0.27657, y = 0.05168, z
53 0.72343 0.05168 0.91352
56 0.77657 0.94832 0.41352
55 0.27657 0.55168 0.58648
54 0.22343 0.44832 0.08648
64 0.91352 0.72343 0.05168
62 0.58648 0.27657 0.55168
63 0.08648 0.22343 0.44832
61 0.41352 0.77657 0.94832
58 0.05168 0.91352 0.72343
57 0.44832 0.08648 0.22343
59 0.94832 0.41352 0.77657
60 0.55168 0.58648 0.27657
For Nitrogen: Wyckoff position a, x = -0.34080
65 0.65920 0.65920 0.65920
68 0.84080 0.34080 0.15920
67 0.34080 0.15920 0.84080
66 0.15920 0.84080 0.34080

100 GPa, Enthalpy: -131.844898 eV
$a, b, c, \alpha, \beta, \gamma$: 6.08633 6.08633 6.08633 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position b, x = 0.12713, y = -0.39977, z
1 0.12713 0.60023 0.54154
13 0.37287 0.39977 0.04154
9 0.87287 0.10023 0.95846
5 0.62713 0.89977 0.45846
45 0.54154 0.12713 0.60023
37 0.95846 0.87287 0.10023
41 0.45846 0.62713 0.89977
33 0.04154 0.37287 0.39977
21 0.60023 0.54154 0.12713
17 0.89977 0.45846 0.62713
25 0.39977 0.04154 0.37287
29 0.10023 0.95846 0.87287
For Hydrogen: Wyckoff position b, x = 0.38539, y = -0.42373, z
2 0.38539 0.57627 0.46484
14 0.11461 0.42373 0.96484
10 0.61461 0.07627 0.03516
6 0.88539 0.92373 0.53516

46 0.46484 0.38539 0.57627
38 0.03516 0.61461 0.07627
42 0.53516 0.88539 0.92373
34 0.96484 0.11461 0.42373
22 0.57627 0.46484 0.38539
18 0.92373 0.53516 0.88539
26 0.42373 0.96484 0.11461
30 0.07627 0.03516 0.61461
For Hydrogen: Wyckoff position b, x = 0.18096, y = -0.36508, z
3 0.18096 0.63492 0.27580
15 0.31904 0.36508 0.77580
11 0.81904 0.13492 0.22420
7 0.68096 0.86508 0.72420
47 0.27580 0.18096 0.63492
39 0.22420 0.81904 0.13492
43 0.72420 0.68096 0.86508
35 0.77580 0.31904 0.36508
23 0.63492 0.27580 0.18096
19 0.86508 0.72420 0.68096
27 0.36508 0.77580 0.31904
31 0.13492 0.22420 0.81904
For Hydrogen: Wyckoff position b, x = 0.11216, y = 0.03391, z
4 0.11216 0.03391 0.26807
16 0.38784 0.96609 0.76807
12 0.88784 0.53391 0.23193
8 0.61216 0.46609 0.73193
48 0.26807 0.11216 0.03391
40 0.23193 0.88784 0.53391
44 0.73193 0.61216 0.46609
36 0.76807 0.38784 0.96609
24 0.03391 0.26807 0.11216
20 0.46609 0.73193 0.61216
28 0.96609 0.76807 0.38784
32 0.53391 0.23193 0.88784
For Lithium: Wyckoff position a, x = 0.31132
49 0.31132 0.31132 0.31132
52 0.18868 0.68868 0.81132
51 0.68868 0.81132 0.18868
50 0.81132 0.18868 0.68868
For Nitrogen: Wyckoff position b, x = 0.22428, y = -0.44447, z
53 0.22428 0.55553 0.41267
56 0.27572 0.44447 0.91267
55 0.77572 0.05553 0.08733
54 0.72428 0.94447 0.58733

64 0.41267 0.22428 0.55553
62 0.08733 0.77572 0.05553
63 0.58733 0.72428 0.94447
61 0.91267 0.27572 0.44447
58 0.55553 0.41267 0.22428
57 0.94447 0.58733 0.72428
59 0.44447 0.91267 0.27572
60 0.05553 0.08733 0.77572
For Nitrogen: Wyckoff position a, x = 0.15410
65 0.15410 0.15410 0.15410
68 0.34590 0.84590 0.65410
67 0.84590 0.65410 0.34590
66 0.65410 0.34590 0.84590

150 GPa, Enthalpy: -66.105256 eV
$a, b, c, \alpha, \beta, \gamma$: 5.82590 5.82590 5.82590 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position b, x = 0.12295, y = -0.39989, z
1 0.12295 0.60011 0.54735
13 0.37705 0.39989 0.04735
9 0.87705 0.10011 0.95265
5 0.62295 0.89989 0.45265
45 0.54735 0.12295 0.60011
37 0.95265 0.87705 0.10011
41 0.45265 0.62295 0.89989
33 0.04735 0.37705 0.39989
21 0.60011 0.54735 0.12295
17 0.89989 0.45265 0.62295
25 0.39989 0.04735 0.37705
29 0.10011 0.95265 0.87705
For Hydrogen: Wyckoff position b, x = 0.39167, y = -0.42418, z
2 0.39167 0.57582 0.46845
14 0.10833 0.42418 0.96845
10 0.60833 0.07582 0.03155
6 0.89167 0.92418 0.53155
46 0.46845 0.39167 0.57582
38 0.03155 0.60833 0.07582
42 0.53155 0.89167 0.92418
34 0.96845 0.10833 0.42418
22 0.57582 0.46845 0.39167
18 0.92418 0.53155 0.89167
26 0.42418 0.96845 0.10833
30 0.07582 0.03155 0.60833
For Hydrogen: Wyckoff position b, x = 0.17880, y = -0.36567, z

3 0.17880 0.63433 0.26692
15 0.32120 0.36567 0.76692
11 0.82120 0.13433 0.23308
7 0.67880 0.86567 0.73308
47 0.26692 0.17880 0.63433
39 0.23308 0.82120 0.13433
43 0.73308 0.67880 0.86567
35 0.76692 0.32120 0.36567
23 0.63433 0.26692 0.17880
19 0.86567 0.73308 0.67880
27 0.36567 0.76692 0.32120
31 0.13433 0.23308 0.82120
For Hydrogen: Wyckoff position b, x = 0.11590, y = 0.02876, z
4 0.11590 0.02876 0.27643
16 0.38410 0.97124 0.77643
12 0.88410 0.52876 0.22357
8 0.61590 0.47124 0.72357
48 0.27643 0.11590 0.02876
40 0.22357 0.88410 0.52876
44 0.72357 0.61590 0.47124
36 0.77643 0.38410 0.97124
24 0.02876 0.27643 0.11590
20 0.47124 0.72357 0.61590
28 0.97124 0.77643 0.38410
32 0.52876 0.22357 0.88410
For Lithium: Wyckoff position a, x = 0.30946
49 0.30946 0.30946 0.30946
52 0.19054 0.69054 0.80946
51 0.69054 0.80946 0.19054
50 0.80946 0.19054 0.69054
For Nitrogen: Wyckoff position b, x = 0.22510, y = -0.44229, z
53 0.22510 0.55771 0.41237
56 0.27490 0.44229 0.91237
55 0.77490 0.05771 0.08763
54 0.72510 0.94229 0.58763
64 0.41237 0.22510 0.55771
62 0.08763 0.77490 0.05771
63 0.58763 0.72510 0.94229
61 0.91237 0.27490 0.44229
58 0.55771 0.41237 0.22510
57 0.94229 0.58763 0.72510
59 0.44229 0.91237 0.27490
60 0.05771 0.08763 0.77490
For Nitrogen: Wyckoff position a, x = 0.15015

65 0.15015 0.15015 0.15015
68 0.34985 0.84985 0.65015
67 0.84985 0.65015 0.34985
66 0.65015 0.34985 0.84985

200 GPa, Enthalpy: -7.338989 eV
$a, b, c, \alpha, \beta, \gamma$: 5.64245 5.64245 5.64245 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position b, x = 0.11940, y = -0.39960, z
1 0.11940 0.60040 0.55143
13 0.38060 0.39960 0.05143
9 0.88060 0.10040 0.94857
5 0.61940 0.89960 0.44857
45 0.55143 0.11940 0.60040
37 0.94857 0.88060 0.10040
41 0.44857 0.61940 0.89960
33 0.05143 0.38060 0.39960
21 0.60040 0.55143 0.11940
17 0.89960 0.44857 0.61940
25 0.39960 0.05143 0.38060
29 0.10040 0.94857 0.88060
For Hydrogen: Wyckoff position b, x = 0.39555, y = -0.42487, z
2 0.39555 0.57513 0.47378
14 0.10445 0.42487 0.97378
10 0.60445 0.07513 0.02622
6 0.89555 0.92487 0.52622
46 0.47378 0.39555 0.57513
38 0.02622 0.60445 0.07513
42 0.52622 0.89555 0.92487
34 0.97378 0.10445 0.42487
22 0.57513 0.47378 0.39555
18 0.92487 0.52622 0.89555
26 0.42487 0.97378 0.10445
30 0.07513 0.02622 0.60445
For Hydrogen: Wyckoff position b, x = 0.17879, y = -0.36793, z
3 0.17879 0.63207 0.25883
15 0.32121 0.36793 0.75883
11 0.82121 0.13207 0.24117
7 0.67879 0.86793 0.74117
47 0.25883 0.17879 0.63207
39 0.24117 0.82121 0.13207
43 0.74117 0.67879 0.86793
35 0.75883 0.32121 0.36793
23 0.63207 0.25883 0.17879

19 0.86793 0.74117 0.67879
27 0.36793 0.75883 0.32121
31 0.13207 0.24117 0.82121
For Hydrogen: Wyckoff position b, x = 0.11870, y = 0.02424, z
4 0.11870 0.02424 0.28049
16 0.38130 0.97576 0.78049
12 0.88130 0.52424 0.21951
8 0.61870 0.47576 0.71951
48 0.28049 0.11870 0.02424
40 0.21951 0.88130 0.52424
44 0.71951 0.61870 0.47576
36 0.78049 0.38130 0.97576
24 0.02424 0.28049 0.11870
20 0.47576 0.71951 0.61870
28 0.97576 0.78049 0.38130
32 0.52424 0.21951 0.88130
For Lithium: Wyckoff position a, x = 0.30849
49 0.30849 0.30849 0.30849
52 0.19151 0.69151 0.80849
51 0.69151 0.80849 0.19151
50 0.80849 0.19151 0.69151
For Nitrogen: Wyckoff position b, x = 0.22564, y = -0.44069, z
53 0.22564 0.55931 0.41228
56 0.27436 0.44069 0.91228
55 0.77436 0.05931 0.08772
54 0.72564 0.94069 0.58772
64 0.41228 0.22564 0.55931
62 0.08772 0.77436 0.05931
63 0.58772 0.72564 0.94069
61 0.91228 0.27436 0.44069
58 0.55931 0.41228 0.22564
57 0.94069 0.58772 0.72564
59 0.44069 0.91228 0.27436
60 0.05931 0.08772 0.77436
For Nitrogen: Wyckoff position a, x = 0.14803
65 0.14803 0.14803 0.14803
68 0.35197 0.85197 0.64803
67 0.85197 0.64803 0.35197
66 0.64803 0.35197 0.85197

2.6 Phase II single point, Space Group 220

0 GPa, Enthalpy: -649.075475 eV
$a, b, c, \alpha, \beta, \gamma$: 14.83679 14.83679 14.83679 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position e, x = -0.22454, y = 0.23710, z
1 0.27546 0.73710 0.67475
13 0.72454 0.23710 0.82525
5 0.27546 0.26290 0.82525
9 0.22454 0.26290 0.17475
21 0.67475 0.27546 0.73710
17 0.82525 0.27546 0.26290
29 0.17475 0.22454 0.26290
25 0.82525 0.72454 0.23710
45 0.73710 0.67475 0.27546
37 0.26290 0.17475 0.22454
33 0.23710 0.82525 0.72454
41 0.26290 0.82525 0.27546
81 0.48710 0.02546 0.42475
85 0.01290 0.02546 0.57525
93 0.48710 0.97454 0.07525
89 0.51290 0.47454 0.42475
77 0.42475 0.48710 0.02546
65 0.07525 0.48710 0.97454
69 0.42475 0.51290 0.47454
73 0.57525 0.01290 0.02546
53 0.02546 0.42475 0.48710
61 0.47454 0.42475 0.51290
49 0.02546 0.57525 0.01290
57 0.97454 0.07525 0.48710
For Hydrogen: Wyckoff position e, x = 0.34560, y = -0.23320, z
2 0.34560 0.76680 0.48860
14 0.65440 0.26680 0.01140
6 0.34560 0.23320 0.01140
10 0.15440 0.23320 0.98860
22 0.48860 0.34560 0.76680
18 0.01140 0.34560 0.23320
30 0.98860 0.15440 0.23320
26 0.01140 0.65440 0.26680
46 0.76680 0.48860 0.34560
38 0.23320 0.98860 0.15440
34 0.26680 0.01140 0.65440
42 0.23320 0.01140 0.34560
82 0.51680 0.09560 0.23860

86 0.98320 0.09560 0.76140
94 0.51680 0.90440 0.26140
90 0.48320 0.40440 0.23860
78 0.23860 0.51680 0.09560
66 0.26140 0.51680 0.90440
70 0.23860 0.48320 0.40440
74 0.76140 0.98320 0.09560
54 0.09560 0.23860 0.51680
62 0.40440 0.23860 0.48320
50 0.09560 0.76140 0.98320
58 0.90440 0.26140 0.51680
For Hydrogen: Wyckoff position e, x = 0.34177, y = -0.13430, z
3 0.34177 0.86570 0.44700
15 0.15823 0.86570 0.55300
7 0.34177 0.13430 0.05300
11 0.15823 0.13430 0.94700
23 0.44700 0.34177 0.86570
19 0.05300 0.34177 0.13430
31 0.94700 0.15823 0.13430
27 0.55300 0.15823 0.86570
47 0.86570 0.44700 0.34177
39 0.13430 0.94700 0.15823
35 0.86570 0.55300 0.15823
43 0.13430 0.05300 0.34177
83 0.61570 0.09177 0.19700
87 0.38430 0.59177 0.30300
95 0.61570 0.90823 0.30300
91 0.38430 0.40823 0.19700
79 0.19700 0.61570 0.09177
67 0.30300 0.61570 0.90823
71 0.19700 0.38430 0.40823
75 0.30300 0.38430 0.59177
55 0.09177 0.19700 0.61570
63 0.40823 0.19700 0.38430
51 0.59177 0.30300 0.38430
59 0.90823 0.30300 0.61570
For Hydrogen: Wyckoff position e, x = 0.43010, y = -0.17634, z
4 0.43010 0.82366 0.46433
16 0.56990 0.32366 0.03567
8 0.43010 0.17634 0.03567
12 0.06990 0.17634 0.96433
24 0.46433 0.43010 0.82366
20 0.03567 0.43010 0.17634
32 0.96433 0.06990 0.17634

28 0.03567 0.56990 0.32366
48 0.82366 0.46433 0.43010
40 0.17634 0.96433 0.06990
36 0.32366 0.03567 0.56990
44 0.17634 0.03567 0.43010
84 0.57366 0.18010 0.21433
88 0.92634 0.18010 0.78567
96 0.57366 0.81990 0.28567
92 0.42634 0.31990 0.21433
80 0.21433 0.57366 0.18010
68 0.28567 0.57366 0.81990
72 0.21433 0.42634 0.31990
76 0.78567 0.92634 0.18010
56 0.18010 0.21433 0.57366
64 0.31990 0.21433 0.42634
52 0.18010 0.78567 0.92634
60 0.81990 0.28567 0.57366
For Lithium: Wyckoff position c, x = 0.12570
97 0.87430 0.37430 0.12570
100 0.12570 0.87430 0.37430
98 0.37430 0.12570 0.87430
99 0.12570 0.12570 0.12570
101 0.12430 0.62430 0.87570
103 0.87570 0.12430 0.62430
102 0.62430 0.87570 0.12430
104 0.37570 0.37570 0.37570
For Nitrogen: Wyckoff position e, x = 0.36993, y = -0.17109, z
105 0.36993 0.82891 0.49330
108 0.63007 0.32891 0.00670
106 0.36993 0.17109 0.00670
107 0.13007 0.17109 0.99330
110 0.49330 0.36993 0.82891
109 0.00670 0.36993 0.17109
112 0.99330 0.13007 0.17109
111 0.00670 0.63007 0.32891
116 0.82891 0.49330 0.36993
114 0.17109 0.99330 0.13007
113 0.32891 0.00670 0.63007
115 0.17109 0.00670 0.36993
125 0.57891 0.11993 0.24330
126 0.92109 0.11993 0.75670
128 0.57891 0.88007 0.25670
127 0.42109 0.38007 0.24330
124 0.24330 0.57891 0.11993

121 0.25670 0.57891 0.88007
122 0.24330 0.42109 0.38007
123 0.75670 0.92109 0.11993
118 0.11993 0.24330 0.57891
120 0.38007 0.24330 0.42109
117 0.11993 0.75670 0.92109
119 0.88007 0.25670 0.57891
For Nitrogen: Wyckoff position c, x = 0.20488
129 0.79512 0.29512 0.20488
132 0.20488 0.79512 0.29512
130 0.29512 0.20488 0.79512
131 0.20488 0.20488 0.20488
133 0.04512 0.54512 0.95488
135 0.95488 0.04512 0.54512
134 0.54512 0.95488 0.04512
136 0.45488 0.45488 0.45488

2.7 Phase II fixed lattice, Space Group 220

0 GPa, Enthalpy: -653.856366 eV
$a, b, c, \alpha, \beta, \gamma$: 14.83679 14.83679 14.83679 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position e, x = -0.22541, y = 0.23453, z
1 0.27459 0.73453 0.67530
13 0.72541 0.23453 0.82470
5 0.27459 0.26547 0.82470
9 0.22541 0.26547 0.17530
21 0.67530 0.27459 0.73453
17 0.82470 0.27459 0.26547
29 0.17530 0.22541 0.26547
25 0.82470 0.72541 0.23453
45 0.73453 0.67530 0.27459
37 0.26547 0.17530 0.22541
33 0.23453 0.82470 0.72541
41 0.26547 0.82470 0.27459
81 0.48453 0.02459 0.42530
85 0.01547 0.02459 0.57470
93 0.48453 0.97541 0.07470
89 0.51547 0.47541 0.42530
77 0.42530 0.48453 0.02459
65 0.07470 0.48453 0.97541
69 0.42530 0.51547 0.47541
73 0.57470 0.01547 0.02459

53 0.02459 0.42530 0.48453
61 0.47541 0.42530 0.51547
49 0.02459 0.57470 0.01547
57 0.97541 0.07470 0.48453
For Hydrogen: Wyckoff position e, x = 0.34462, y = -0.23658, z
2 0.34462 0.76342 0.48402
14 0.65538 0.26342 0.01598
6 0.34462 0.23658 0.01598
10 0.15538 0.23658 0.98402
22 0.48402 0.34462 0.76342
18 0.01598 0.34462 0.23658
30 0.98402 0.15538 0.23658
26 0.01598 0.65538 0.26342
46 0.76342 0.48402 0.34462
38 0.23658 0.98402 0.15538
34 0.26342 0.01598 0.65538
42 0.23658 0.01598 0.34462
82 0.51342 0.09462 0.23402
86 0.98658 0.09462 0.76598
94 0.51342 0.90538 0.26598
90 0.48658 0.40538 0.23402
78 0.23402 0.51342 0.09462
66 0.26598 0.51342 0.90538
70 0.23402 0.48658 0.40538
74 0.76598 0.98658 0.09462
54 0.09462 0.23402 0.51342
62 0.40538 0.23402 0.48658
50 0.09462 0.76598 0.98658
58 0.90538 0.26598 0.51342
For Hydrogen: Wyckoff position e, x = 0.33777, y = -0.13282, z
3 0.33777 0.86718 0.44623
15 0.16223 0.86718 0.55377
7 0.33777 0.13282 0.05377
11 0.16223 0.13282 0.94623
23 0.44623 0.33777 0.86718
19 0.05377 0.33777 0.13282
31 0.94623 0.16223 0.13282
27 0.55377 0.16223 0.86718
47 0.86718 0.44623 0.33777
39 0.13282 0.94623 0.16223
35 0.86718 0.55377 0.16223
43 0.13282 0.05377 0.33777
83 0.61718 0.08777 0.19623
87 0.38282 0.58777 0.30377

95 0.61718 0.91223 0.30377
91 0.38282 0.41223 0.19623
79 0.19623 0.61718 0.08777
67 0.30377 0.61718 0.91223
71 0.19623 0.38282 0.41223
75 0.30377 0.38282 0.58777
55 0.08777 0.19623 0.61718
63 0.41223 0.19623 0.38282
51 0.58777 0.30377 0.38282
59 0.91223 0.30377 0.61718
For Hydrogen: Wyckoff position e, x = 0.43602, y = -0.17883, z
4 0.43602 0.82117 0.46255
16 0.56398 0.32117 0.03745
8 0.43602 0.17883 0.03745
12 0.06398 0.17883 0.96255
24 0.46255 0.43602 0.82117
20 0.03745 0.43602 0.17883
32 0.96255 0.06398 0.17883
28 0.03745 0.56398 0.32117
48 0.82117 0.46255 0.43602
40 0.17883 0.96255 0.06398
36 0.32117 0.03745 0.56398
44 0.17883 0.03745 0.43602
84 0.57117 0.18602 0.21255
88 0.92883 0.18602 0.78745
96 0.57117 0.81398 0.28745
92 0.42883 0.31398 0.21255
80 0.21255 0.57117 0.18602
68 0.28745 0.57117 0.81398
72 0.21255 0.42883 0.31398
76 0.78745 0.92883 0.18602
56 0.18602 0.21255 0.57117
64 0.31398 0.21255 0.42883
52 0.18602 0.78745 0.92883
60 0.81398 0.28745 0.57117
For Lithium: Wyckoff position c, x = 0.12403
97 0.87597 0.37597 0.12403
100 0.12403 0.87597 0.37597
98 0.37597 0.12403 0.87597
99 0.12403 0.12403 0.12403
101 0.12597 0.62597 0.87403
103 0.87403 0.12597 0.62597
102 0.62597 0.87403 0.12597
104 0.37403 0.37403 0.37403

For Nitrogen: Wyckoff position e, x = 0.37274, y = -0.17335, z
105 0.37274 0.82665 0.49032
108 0.62726 0.32665 0.00968
106 0.37274 0.17335 0.00968
107 0.12726 0.17335 0.99032
110 0.49032 0.37274 0.82665
109 0.00968 0.37274 0.17335
112 0.99032 0.12726 0.17335
111 0.00968 0.62726 0.32665
116 0.82665 0.49032 0.37274
114 0.17335 0.99032 0.12726
113 0.32665 0.00968 0.62726
115 0.17335 0.00968 0.37274
125 0.57665 0.12274 0.24032
126 0.92335 0.12274 0.75968
128 0.57665 0.87726 0.25968
127 0.42335 0.37726 0.24032
124 0.24032 0.57665 0.12274
121 0.25968 0.57665 0.87726
122 0.24032 0.42335 0.37726
123 0.75968 0.92335 0.12274
118 0.12274 0.24032 0.57665
120 0.37726 0.24032 0.42335
117 0.12274 0.75968 0.92335
119 0.87726 0.25968 0.57665
For Nitrogen: Wyckoff position c, x = 0.20641
129 0.79359 0.29359 0.20641
132 0.20641 0.79359 0.29359
130 0.29359 0.20641 0.79359
131 0.20641 0.20641 0.20641
133 0.04359 0.54359 0.95641
135 0.95641 0.04359 0.54359
134 0.54359 0.95641 0.04359
136 0.45641 0.45641 0.45641

2.8 Phase II optimized, Space Group 220

0 GPa, Enthalpy: -654.000434 eV
$a, b, c, \alpha, \beta, \gamma$: 15.19359 15.19359 15.19359 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position e, x = -0.22326, y = 0.23661, z
1 0.27674 0.73661 0.67533
13 0.72326 0.23661 0.82467

5 0.27674 0.26339 0.82467
9 0.22326 0.26339 0.17533
21 0.67533 0.27674 0.73661
17 0.82467 0.27674 0.26339
29 0.17533 0.22326 0.26339
25 0.82467 0.72326 0.23661
45 0.73661 0.67533 0.27674
37 0.26339 0.17533 0.22326
33 0.23661 0.82467 0.72326
41 0.26339 0.82467 0.27674
81 0.48661 0.02674 0.42533
85 0.01339 0.02674 0.57467
93 0.48661 0.97326 0.07467
89 0.51339 0.47326 0.42533
77 0.42533 0.48661 0.02674
65 0.07467 0.48661 0.97326
69 0.42533 0.51339 0.47326
73 0.57467 0.01339 0.02674
53 0.02674 0.42533 0.48661
61 0.47326 0.42533 0.51339
49 0.02674 0.57467 0.01339
57 0.97326 0.07467 0.48661
For Hydrogen: Wyckoff position e, x = 0.34691, y = -0.23657, z
2 0.34691 0.76343 0.48858
14 0.65309 0.26343 0.01142
6 0.34691 0.23657 0.01142
10 0.15309 0.23657 0.98858
22 0.48858 0.34691 0.76343
18 0.01142 0.34691 0.23657
30 0.98858 0.15309 0.23657
26 0.01142 0.65309 0.26343
46 0.76343 0.48858 0.34691
38 0.23657 0.98858 0.15309
34 0.26343 0.01142 0.65309
42 0.23657 0.01142 0.34691
82 0.51343 0.09691 0.23858
86 0.98657 0.09691 0.76142
94 0.51343 0.90309 0.26142
90 0.48657 0.40309 0.23858
78 0.23858 0.51343 0.09691
66 0.26142 0.51343 0.90309
70 0.23858 0.48657 0.40309
74 0.76142 0.98657 0.09691
54 0.09691 0.23858 0.51343

62 0.40309 0.23858 0.48657
50 0.09691 0.76142 0.98657
58 0.90309 0.26142 0.51343
For Hydrogen: Wyckoff position e, x = 0.34266, y = -0.13585, z
3 0.34266 0.86415 0.45007
15 0.15734 0.86415 0.54993
7 0.34266 0.13585 0.04993
11 0.15734 0.13585 0.95007
23 0.45007 0.34266 0.86415
19 0.04993 0.34266 0.13585
31 0.95007 0.15734 0.13585
27 0.54993 0.15734 0.86415
47 0.86415 0.45007 0.34266
39 0.13585 0.95007 0.15734
35 0.86415 0.54993 0.15734
43 0.13585 0.04993 0.34266
83 0.61415 0.09266 0.20007
87 0.38585 0.59266 0.29993
95 0.61415 0.90734 0.29993
91 0.38585 0.40734 0.20007
79 0.20007 0.61415 0.09266
67 0.29993 0.61415 0.90734
71 0.20007 0.38585 0.40734
75 0.29993 0.38585 0.59266
55 0.09266 0.20007 0.61415
63 0.40734 0.20007 0.38585
51 0.59266 0.29993 0.38585
59 0.90734 0.29993 0.61415
For Hydrogen: Wyckoff position e, x = 0.43750, y = -0.18186, z
4 0.43750 0.81814 0.46908
16 0.56250 0.31814 0.03092
8 0.43750 0.18186 0.03092
12 0.06250 0.18186 0.96908
24 0.46908 0.43750 0.81814
20 0.03092 0.43750 0.18186
32 0.96908 0.06250 0.18186
28 0.03092 0.56250 0.31814
48 0.81814 0.46908 0.43750
40 0.18186 0.96908 0.06250
36 0.31814 0.03092 0.56250
44 0.18186 0.03092 0.43750
84 0.56814 0.18750 0.21908
88 0.93186 0.18750 0.78092
96 0.56814 0.81250 0.28092

92 0.43186 0.31250 0.21908
80 0.21908 0.56814 0.18750
68 0.28092 0.56814 0.81250
72 0.21908 0.43186 0.31250
76 0.78092 0.93186 0.18750
56 0.18750 0.21908 0.56814
64 0.31250 0.21908 0.43186
52 0.18750 0.78092 0.93186
60 0.81250 0.28092 0.56814
For Lithium: Wyckoff position c, x = 0.12478
97 0.87522 0.37522 0.12478
100 0.12478 0.87522 0.37522
98 0.37522 0.12478 0.87522
99 0.12478 0.12478 0.12478
101 0.12522 0.62522 0.87478
103 0.87478 0.12522 0.62522
102 0.62522 0.87478 0.12522
104 0.37478 0.37478 0.37478
For Nitrogen: Wyckoff position e, x = 0.37514, y = -0.17518, z
105 0.37514 0.82482 0.49458
108 0.62486 0.32482 0.00542
106 0.37514 0.17518 0.00542
107 0.12486 0.17518 0.99458
110 0.49458 0.37514 0.82482
109 0.00542 0.37514 0.17518
112 0.99458 0.12486 0.17518
111 0.00542 0.62486 0.32482
116 0.82482 0.49458 0.37514
114 0.17518 0.99458 0.12486
113 0.32482 0.00542 0.62486
115 0.17518 0.00542 0.37514
125 0.57482 0.12514 0.24458
126 0.92518 0.12514 0.75542
128 0.57482 0.87486 0.25542
127 0.42518 0.37486 0.24458
124 0.24458 0.57482 0.12514
121 0.25542 0.57482 0.87486
122 0.24458 0.42518 0.37486
123 0.75542 0.92518 0.12514
118 0.12514 0.24458 0.57482
120 0.37486 0.24458 0.42518
117 0.12514 0.75542 0.92518
119 0.87486 0.25542 0.57482
For Nitrogen: Wyckoff position c, x = 0.20534

129 0.79466 0.29466 0.20534
132 0.20534 0.79466 0.29466
130 0.29466 0.20534 0.79466
131 0.20534 0.20534 0.20534
133 0.04466 0.54466 0.95534
135 0.95534 0.04466 0.54466
134 0.54466 0.95534 0.04466
136 0.45534 0.45534 0.45534

50 GPa, Enthalpy: -425.358685 eV
$a, b, c, \alpha, \beta, \gamma$: 10.28218 10.28218 10.28218 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position e, x = -0.25707, y = 0.18363, z
1 0.74293 0.18363 0.18423
13 0.25707 0.68363 0.31577
5 0.24293 0.31637 0.81577
9 0.25707 0.31637 0.18423
21 0.18423 0.74293 0.18363
17 0.81577 0.24293 0.31637
29 0.18423 0.25707 0.31637
25 0.31577 0.25707 0.68363
45 0.18363 0.18423 0.74293
37 0.31637 0.18423 0.25707
33 0.68363 0.31577 0.25707
41 0.31637 0.81577 0.24293
81 0.43363 0.99293 0.43423
85 0.06637 0.99293 0.56577
93 0.43363 0.00707 0.06577
89 0.56637 0.50707 0.43423
77 0.43423 0.43363 0.99293
65 0.06577 0.43363 0.00707
69 0.43423 0.56637 0.50707
73 0.56577 0.06637 0.99293
53 0.99293 0.43423 0.43363
61 0.50707 0.43423 0.56637
49 0.99293 0.56577 0.06637
57 0.00707 0.06577 0.43363
For Hydrogen: Wyckoff position e, x = 0.32888, y = -0.29755, z
2 0.32888 0.70245 0.47330
14 0.67112 0.20245 0.02670
6 0.32888 0.29755 0.02670
10 0.17112 0.29755 0.97330
22 0.47330 0.32888 0.70245
18 0.02670 0.32888 0.29755

30 0.97330 0.17112 0.29755
26 0.02670 0.67112 0.20245
46 0.70245 0.47330 0.32888
38 0.29755 0.97330 0.17112
34 0.20245 0.02670 0.67112
42 0.29755 0.02670 0.32888
82 0.45245 0.07888 0.22330
86 0.04755 0.07888 0.77670
94 0.45245 0.92112 0.27670
90 0.54755 0.42112 0.22330
78 0.22330 0.45245 0.07888
66 0.27670 0.45245 0.92112
70 0.22330 0.54755 0.42112
74 0.77670 0.04755 0.07888
54 0.07888 0.22330 0.45245
62 0.42112 0.22330 0.54755
50 0.07888 0.77670 0.04755
58 0.92112 0.27670 0.45245
For Hydrogen: Wyckoff position e, x = 0.31311, y = -0.14151, z
3 0.31311 0.85849 0.41758
15 0.18689 0.85849 0.58242
7 0.31311 0.14151 0.08242
11 0.18689 0.14151 0.91758
23 0.41758 0.31311 0.85849
19 0.08242 0.31311 0.14151
31 0.91758 0.18689 0.14151
27 0.58242 0.18689 0.85849
47 0.85849 0.41758 0.31311
39 0.14151 0.91758 0.18689
35 0.85849 0.58242 0.18689
43 0.14151 0.08242 0.31311
83 0.60849 0.06311 0.16758
87 0.39151 0.56311 0.33242
95 0.60849 0.93689 0.33242
91 0.39151 0.43689 0.16758
79 0.16758 0.60849 0.06311
67 0.33242 0.60849 0.93689
71 0.16758 0.39151 0.43689
75 0.33242 0.39151 0.56311
55 0.06311 0.16758 0.60849
63 0.43689 0.16758 0.39151
51 0.56311 0.33242 0.39151
59 0.93689 0.33242 0.60849
For Hydrogen: Wyckoff position e, x = 0.45927, y = -0.19186, z

4 0.45927 0.80814 0.44032
16 0.54073 0.30814 0.05968
8 0.45927 0.19186 0.05968
12 0.54073 0.69186 0.44032
24 0.44032 0.45927 0.80814
20 0.05968 0.45927 0.19186
32 0.44032 0.54073 0.69186
28 0.05968 0.54073 0.30814
48 0.80814 0.44032 0.45927
40 0.69186 0.44032 0.54073
36 0.30814 0.05968 0.54073
44 0.19186 0.05968 0.45927
84 0.55814 0.20927 0.19032
88 0.44186 0.70927 0.30968
96 0.55814 0.79073 0.30968
92 0.44186 0.29073 0.19032
80 0.19032 0.55814 0.20927
68 0.30968 0.55814 0.79073
72 0.19032 0.44186 0.29073
76 0.30968 0.44186 0.70927
56 0.20927 0.19032 0.55814
64 0.29073 0.19032 0.44186
52 0.70927 0.30968 0.44186
60 0.79073 0.30968 0.55814
For Lithium: Wyckoff position c, x = 0.13166
97 0.86834 0.36834 0.13166
100 0.13166 0.86834 0.36834
98 0.36834 0.13166 0.86834
99 0.13166 0.13166 0.13166
101 0.11834 0.61834 0.88166
103 0.88166 0.11834 0.61834
102 0.61834 0.88166 0.11834
104 0.38166 0.38166 0.38166
For Nitrogen: Wyckoff position e, x = 0.36842, y = -0.20069, z
105 0.36842 0.79931 0.47395
108 0.63158 0.29931 0.02605
106 0.36842 0.20069 0.02605
107 0.13158 0.20069 0.97395
110 0.47395 0.36842 0.79931
109 0.02605 0.36842 0.20069
112 0.97395 0.13158 0.20069
111 0.02605 0.63158 0.29931
116 0.79931 0.47395 0.36842
114 0.20069 0.97395 0.13158

113 0.29931 0.02605 0.63158
115 0.20069 0.02605 0.36842
125 0.54931 0.11842 0.22395
126 0.95069 0.11842 0.77605
128 0.54931 0.88158 0.27605
127 0.45069 0.38158 0.22395
124 0.22395 0.54931 0.11842
121 0.27605 0.54931 0.88158
122 0.22395 0.45069 0.38158
123 0.77605 0.95069 0.11842
118 0.11842 0.22395 0.54931
120 0.38158 0.22395 0.45069
117 0.11842 0.77605 0.95069
119 0.88158 0.27605 0.54931
For Nitrogen: Wyckoff position c, x = 0.23382
129 0.76618 0.26618 0.23382
132 0.23382 0.76618 0.26618
130 0.26618 0.23382 0.76618
131 0.23382 0.23382 0.23382
133 0.01618 0.51618 0.98382
135 0.98382 0.01618 0.51618
134 0.51618 0.98382 0.01618
136 0.48382 0.48382 0.48382

100 GPa, Enthalpy: -274.034828 eV
$a, b, c, \alpha, \beta, \gamma$: 9.57782 9.57782 9.57782 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position e, x = -0.25680, y = 0.17628, z
1 0.74320 0.17628 0.18270
13 0.25680 0.67628 0.31730
5 0.24320 0.32372 0.81730
9 0.25680 0.32372 0.18270
21 0.18270 0.74320 0.17628
17 0.81730 0.24320 0.32372
29 0.18270 0.25680 0.32372
25 0.31730 0.25680 0.67628
45 0.17628 0.18270 0.74320
37 0.32372 0.18270 0.25680
33 0.67628 0.31730 0.25680
41 0.32372 0.81730 0.24320
81 0.42628 0.99320 0.43270
85 0.07372 0.99320 0.56730
93 0.42628 0.00680 0.06730
89 0.57372 0.50680 0.43270

77 0.43270 0.42628 0.99320
65 0.06730 0.42628 0.00680
69 0.43270 0.57372 0.50680
73 0.56730 0.07372 0.99320
53 0.99320 0.43270 0.42628
61 0.50680 0.43270 0.57372
49 0.99320 0.56730 0.07372
57 0.00680 0.06730 0.42628
For Hydrogen: Wyckoff position e, x = 0.32280, y = -0.31145, z
2 0.32280 0.68855 0.47542
14 0.67720 0.18855 0.02458
6 0.32280 0.31145 0.02458
10 0.17720 0.31145 0.97542
22 0.47542 0.32280 0.68855
18 0.02458 0.32280 0.31145
30 0.97542 0.17720 0.31145
26 0.02458 0.67720 0.18855
46 0.68855 0.47542 0.32280
38 0.31145 0.97542 0.17720
34 0.18855 0.02458 0.67720
42 0.31145 0.02458 0.32280
82 0.43855 0.07280 0.22542
86 0.06145 0.07280 0.77458
94 0.43855 0.92720 0.27458
90 0.56145 0.42720 0.22542
78 0.22542 0.43855 0.07280
66 0.27458 0.43855 0.92720
70 0.22542 0.56145 0.42720
74 0.77458 0.06145 0.07280
54 0.07280 0.22542 0.43855
62 0.42720 0.22542 0.56145
50 0.07280 0.77458 0.06145
58 0.92720 0.27458 0.43855
For Hydrogen: Wyckoff position e, x = 0.30515, y = -0.13888, z
3 0.30515 0.86112 0.43018
15 0.19485 0.86112 0.56982
7 0.30515 0.13888 0.06982
11 0.19485 0.13888 0.93018
23 0.43018 0.30515 0.86112
19 0.06982 0.30515 0.13888
31 0.93018 0.19485 0.13888
27 0.56982 0.19485 0.86112
47 0.86112 0.43018 0.30515
39 0.13888 0.93018 0.19485

35 0.86112 0.56982 0.19485
43 0.13888 0.06982 0.30515
83 0.61112 0.05515 0.18018
87 0.38888 0.55515 0.31982
95 0.61112 0.94485 0.31982
91 0.38888 0.44485 0.18018
79 0.18018 0.61112 0.05515
67 0.31982 0.61112 0.94485
71 0.18018 0.38888 0.44485
75 0.31982 0.38888 0.55515
55 0.05515 0.18018 0.61112
63 0.44485 0.18018 0.38888
51 0.55515 0.31982 0.38888
59 0.94485 0.31982 0.61112
For Hydrogen: Wyckoff position e, x = 0.46348, y = -0.18579, z
4 0.46348 0.81421 0.43377
16 0.53652 0.31421 0.06623
8 0.46348 0.18579 0.06623
12 0.53652 0.68579 0.43377
24 0.43377 0.46348 0.81421
20 0.06623 0.46348 0.18579
32 0.43377 0.53652 0.68579
28 0.06623 0.53652 0.31421
48 0.81421 0.43377 0.46348
40 0.68579 0.43377 0.53652
36 0.31421 0.06623 0.53652
44 0.18579 0.06623 0.46348
84 0.56421 0.21348 0.18377
88 0.43579 0.71348 0.31623
96 0.56421 0.78652 0.31623
92 0.43579 0.28652 0.18377
80 0.18377 0.56421 0.21348
68 0.31623 0.56421 0.78652
72 0.18377 0.43579 0.28652
76 0.31623 0.43579 0.71348
56 0.21348 0.18377 0.56421
64 0.28652 0.18377 0.43579
52 0.71348 0.31623 0.43579
60 0.78652 0.31623 0.56421
For Lithium: Wyckoff position c, x = 0.13240
97 0.86760 0.36760 0.13240
100 0.13240 0.86760 0.36760
98 0.36760 0.13240 0.86760
99 0.13240 0.13240 0.13240

101 0.11760 0.61760 0.88240
103 0.88240 0.11760 0.61760
102 0.61760 0.88240 0.11760
104 0.38240 0.38240 0.38240
For Nitrogen: Wyckoff position e, x = 0.37112, y = -0.20793, z
105 0.37112 0.79207 0.47471
108 0.62888 0.29207 0.02529
106 0.37112 0.20793 0.02529
107 0.12888 0.20793 0.97471
110 0.47471 0.37112 0.79207
109 0.02529 0.37112 0.20793
112 0.97471 0.12888 0.20793
111 0.02529 0.62888 0.29207
116 0.79207 0.47471 0.37112
114 0.20793 0.97471 0.12888
113 0.29207 0.02529 0.62888
115 0.20793 0.02529 0.37112
125 0.54207 0.12112 0.22471
126 0.95793 0.12112 0.77529
128 0.54207 0.87888 0.27529
127 0.45793 0.37888 0.22471
124 0.22471 0.54207 0.12112
121 0.27529 0.54207 0.87888
122 0.22471 0.45793 0.37888
123 0.77529 0.95793 0.12112
118 0.12112 0.22471 0.54207
120 0.37888 0.22471 0.45793
117 0.12112 0.77529 0.95793
119 0.87888 0.27529 0.54207
For Nitrogen: Wyckoff position c, x = 0.23612
129 0.76388 0.26388 0.23612
132 0.23612 0.76388 0.26388
130 0.26388 0.23612 0.76388
131 0.23612 0.23612 0.23612
133 0.01388 0.51388 0.98612
135 0.98612 0.01388 0.51388
134 0.51388 0.98612 0.01388
136 0.48612 0.48612 0.48612

150 GPa, Enthalpy: -145.991521 eV
$a, b, c, \alpha, \beta, \gamma$: 9.16986 9.16986 9.16986 90.00000 90.00000 90.00000
For Hydrogen: Wyckoff position e, x = -0.25672, y = 0.17086, z
1 0.74328 0.17086 0.18349
13 0.25672 0.67086 0.31651

5 0.24328 0.32914 0.81651
9 0.25672 0.32914 0.18349
21 0.18349 0.74328 0.17086
17 0.81651 0.24328 0.32914
29 0.18349 0.25672 0.32914
25 0.31651 0.25672 0.67086
45 0.17086 0.18349 0.74328
37 0.32914 0.18349 0.25672
33 0.67086 0.31651 0.25672
41 0.32914 0.81651 0.24328
81 0.42086 0.99328 0.43349
85 0.07914 0.99328 0.56651
93 0.42086 0.00672 0.06651
89 0.57914 0.50672 0.43349
77 0.43349 0.42086 0.99328
65 0.06651 0.42086 0.00672
69 0.43349 0.57914 0.50672
73 0.56651 0.07914 0.99328
53 0.99328 0.43349 0.42086
61 0.50672 0.43349 0.57914
49 0.99328 0.56651 0.07914
57 0.00672 0.06651 0.42086
For Hydrogen: Wyckoff position e, x = 0.31729, y = -0.31941, z
2 0.81729 0.18059 0.97750
14 0.68271 0.18059 0.02250
6 0.31729 0.31941 0.02250
10 0.18271 0.31941 0.97750
22 0.97750 0.81729 0.18059
18 0.02250 0.31729 0.31941
30 0.97750 0.18271 0.31941
26 0.02250 0.68271 0.18059
46 0.18059 0.97750 0.81729
38 0.31941 0.97750 0.18271
34 0.18059 0.02250 0.68271
42 0.31941 0.02250 0.31729
82 0.43059 0.06729 0.22750
86 0.06941 0.06729 0.77250
94 0.43059 0.93271 0.27250
90 0.06941 0.93271 0.72750
78 0.22750 0.43059 0.06729
66 0.27250 0.43059 0.93271
70 0.72750 0.06941 0.93271
74 0.77250 0.06941 0.06729
54 0.06729 0.22750 0.43059

62 0.93271 0.72750 0.06941
50 0.06729 0.77250 0.06941
58 0.93271 0.27250 0.43059
For Hydrogen: Wyckoff position e, x = 0.30237, y = -0.13848, z
3 0.30237 0.86152 0.43639
15 0.19763 0.86152 0.56361
7 0.30237 0.13848 0.06361
11 0.19763 0.13848 0.93639
23 0.43639 0.30237 0.86152
19 0.06361 0.30237 0.13848
31 0.93639 0.19763 0.13848
27 0.56361 0.19763 0.86152
47 0.86152 0.43639 0.30237
39 0.13848 0.93639 0.19763
35 0.86152 0.56361 0.19763
43 0.13848 0.06361 0.30237
83 0.61152 0.05237 0.18639
87 0.38848 0.55237 0.31361
95 0.61152 0.94763 0.31361
91 0.38848 0.44763 0.18639
79 0.18639 0.61152 0.05237
67 0.31361 0.61152 0.94763
71 0.18639 0.38848 0.44763
75 0.31361 0.38848 0.55237
55 0.05237 0.18639 0.61152
63 0.44763 0.18639 0.38848
51 0.55237 0.31361 0.38848
59 0.94763 0.31361 0.61152
For Hydrogen: Wyckoff position e, x = 0.46546, y = -0.18144, z
4 0.46546 0.81856 0.42930
16 0.53454 0.31856 0.07070
8 0.46546 0.18144 0.07070
12 0.53454 0.68144 0.42930
24 0.42930 0.46546 0.81856
20 0.07070 0.46546 0.18144
32 0.42930 0.53454 0.68144
28 0.07070 0.53454 0.31856
48 0.81856 0.42930 0.46546
40 0.68144 0.42930 0.53454
36 0.31856 0.07070 0.53454
44 0.18144 0.07070 0.46546
84 0.56856 0.21546 0.17930
88 0.43144 0.71546 0.32070
96 0.56856 0.78454 0.32070

92 0.43144 0.28454 0.17930
80 0.17930 0.56856 0.21546
68 0.32070 0.56856 0.78454
72 0.17930 0.43144 0.28454
76 0.32070 0.43144 0.71546
56 0.21546 0.17930 0.56856
64 0.28454 0.17930 0.43144
52 0.71546 0.32070 0.43144
60 0.78454 0.32070 0.56856
For Lithium: Wyckoff position c, x = 0.13269
97 0.86731 0.36731 0.13269
100 0.13269 0.86731 0.36731
98 0.36731 0.13269 0.86731
99 0.13269 0.13269 0.13269
101 0.11731 0.61731 0.88269
103 0.88269 0.11731 0.61731
102 0.61731 0.88269 0.11731
104 0.38269 0.38269 0.38269
For Nitrogen: Wyckoff position e, x = 0.37334, y = -0.21284, z
105 0.37334 0.78716 0.47525
108 0.62666 0.28716 0.02475
106 0.37334 0.21284 0.02475
107 0.12666 0.21284 0.97525
110 0.47525 0.37334 0.78716
109 0.02475 0.37334 0.21284
112 0.97525 0.12666 0.21284
111 0.02475 0.62666 0.28716
116 0.78716 0.47525 0.37334
114 0.21284 0.97525 0.12666
113 0.28716 0.02475 0.62666
115 0.21284 0.02475 0.37334
125 0.53716 0.12334 0.22525
126 0.96284 0.12334 0.77475
128 0.53716 0.87666 0.27475
127 0.46284 0.37666 0.22525
124 0.22525 0.53716 0.12334
121 0.27475 0.53716 0.87666
122 0.22525 0.46284 0.37666
123 0.77475 0.96284 0.12334
118 0.12334 0.22525 0.53716
120 0.37666 0.22525 0.46284
117 0.12334 0.77475 0.96284
119 0.87666 0.27475 0.53716
For Nitrogen: Wyckoff position c, x = 0.23755

129 0.76245 0.26245 0.23755
132 0.23755 0.76245 0.26245
130 0.26245 0.23755 0.76245
131 0.23755 0.23755 0.23755
133 0.01245 0.51245 0.98755
135 0.98755 0.01245 0.51245
134 0.51245 0.98755 0.01245
136 0.48755 0.48755 0.48755

200 GPa, Enthalpy: -31.264860 eV
$a, b, c, \alpha, \beta, \gamma$: 8.89014 8.89014 8.89014 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position e, x = -0.25561, y = 0.16851, z
1 0.74439 0.16851 0.18184
13 0.25561 0.66851 0.31816
5 0.24439 0.33149 0.81816
9 0.25561 0.33149 0.18184
21 0.18184 0.74439 0.16851
17 0.81816 0.24439 0.33149
29 0.18184 0.25561 0.33149
25 0.31816 0.25561 0.66851
45 0.16851 0.18184 0.74439
37 0.33149 0.18184 0.25561
33 0.66851 0.31816 0.25561
41 0.33149 0.81816 0.24439
81 0.41851 0.99439 0.43184
85 0.08149 0.99439 0.56816
93 0.41851 0.00561 0.06816
89 0.58149 0.50561 0.43184
77 0.43184 0.41851 0.99439
65 0.06816 0.41851 0.00561
69 0.43184 0.58149 0.50561
73 0.56816 0.08149 0.99439
53 0.99439 0.43184 0.41851
61 0.50561 0.43184 0.58149
49 0.99439 0.56816 0.08149
57 0.00561 0.06816 0.41851
For Hydrogen: Wyckoff position e, x = 0.31532, y = -0.32152, z
2 0.81532 0.17848 0.97736
14 0.68468 0.17848 0.02264
6 0.31532 0.32152 0.02264
10 0.18468 0.32152 0.97736
22 0.97736 0.81532 0.17848
18 0.02264 0.31532 0.32152

30 0.97736 0.18468 0.32152
26 0.02264 0.68468 0.17848
46 0.17848 0.97736 0.81532
38 0.32152 0.97736 0.18468
34 0.17848 0.02264 0.68468
42 0.32152 0.02264 0.31532
82 0.42848 0.06532 0.22736
86 0.07152 0.06532 0.77264
94 0.42848 0.93468 0.27264
90 0.07152 0.93468 0.72736
78 0.22736 0.42848 0.06532
66 0.27264 0.42848 0.93468
70 0.72736 0.07152 0.93468
74 0.77264 0.07152 0.06532
54 0.06532 0.22736 0.42848
62 0.93468 0.72736 0.07152
50 0.06532 0.77264 0.07152
58 0.93468 0.27264 0.42848
For Hydrogen: Wyckoff position e, x = 0.30120, y = -0.13467, z
3 0.30120 0.86533 0.43788
15 0.19880 0.86533 0.56212
7 0.30120 0.13467 0.06212
11 0.19880 0.13467 0.93788
23 0.43788 0.30120 0.86533
19 0.06212 0.30120 0.13467
31 0.93788 0.19880 0.13467
27 0.56212 0.19880 0.86533
47 0.86533 0.43788 0.30120
39 0.13467 0.93788 0.19880
35 0.86533 0.56212 0.19880
43 0.13467 0.06212 0.30120
83 0.61533 0.05120 0.18788
87 0.38467 0.55120 0.31212
95 0.61533 0.94880 0.31212
91 0.38467 0.44880 0.18788
79 0.18788 0.61533 0.05120
67 0.31212 0.61533 0.94880
71 0.18788 0.38467 0.44880
75 0.31212 0.38467 0.55120
55 0.05120 0.18788 0.61533
63 0.44880 0.18788 0.38467
51 0.55120 0.31212 0.38467
59 0.94880 0.31212 0.61533
For Hydrogen: Wyckoff position e, x = 0.46709, y = -0.17809, z

4 0.46709 0.82191 0.42632
16 0.53291 0.32191 0.07368
8 0.46709 0.17809 0.07368
12 0.53291 0.67809 0.42632
24 0.42632 0.46709 0.82191
20 0.07368 0.46709 0.17809
32 0.42632 0.53291 0.67809
28 0.07368 0.53291 0.32191
48 0.82191 0.42632 0.46709
40 0.67809 0.42632 0.53291
36 0.32191 0.07368 0.53291
44 0.17809 0.07368 0.46709
84 0.57191 0.21709 0.17632
88 0.42809 0.71709 0.32368
96 0.57191 0.78291 0.32368
92 0.42809 0.28291 0.17632
80 0.17632 0.57191 0.21709
68 0.32368 0.57191 0.78291
72 0.17632 0.42809 0.28291
76 0.32368 0.42809 0.71709
56 0.21709 0.17632 0.57191
64 0.28291 0.17632 0.42809
52 0.71709 0.32368 0.42809
60 0.78291 0.32368 0.57191
For Lithium: Wyckoff position c, x = 0.13228
97 0.86772 0.36772 0.13228
100 0.13228 0.86772 0.36772
98 0.36772 0.13228 0.86772
99 0.13228 0.13228 0.13228
101 0.11772 0.61772 0.88228
103 0.88228 0.11772 0.61772
102 0.61772 0.88228 0.11772
104 0.38228 0.38228 0.38228
For Nitrogen: Wyckoff position e, x = 0.37389, y = -0.21322, z
105 0.37389 0.78678 0.47459
108 0.62611 0.28678 0.02541
106 0.37389 0.21322 0.02541
107 0.12611 0.21322 0.97459
110 0.47459 0.37389 0.78678
109 0.02541 0.37389 0.21322
112 0.97459 0.12611 0.21322
111 0.02541 0.62611 0.28678
116 0.78678 0.47459 0.37389
114 0.21322 0.97459 0.12611

113 0.28678 0.02541 0.62611
115 0.21322 0.02541 0.37389
125 0.53678 0.12389 0.22459
126 0.96322 0.12389 0.77541
128 0.53678 0.87611 0.27541
127 0.46322 0.37611 0.22459
124 0.22459 0.53678 0.12389
121 0.27541 0.53678 0.87611
122 0.22459 0.46322 0.37611
123 0.77541 0.96322 0.12389
118 0.12389 0.22459 0.53678
120 0.37611 0.22459 0.46322
117 0.12389 0.77541 0.96322
119 0.87611 0.27541 0.53678
For Nitrogen: Wyckoff position c, x = 0.23766
129 0.76234 0.26234 0.23766
132 0.23766 0.76234 0.26234
130 0.26234 0.23766 0.76234
131 0.23766 0.23766 0.23766
133 0.01234 0.51234 0.98766
135 0.98766 0.01234 0.51234
134 0.51234 0.98766 0.01234
136 0.48766 0.48766 0.48766

2.9 Phase III single point, Space Group 198

0 GPa, Enthalpy: -1283.098330 eV
$a, b, c, \alpha, \beta, \gamma$: 14.78342 14.78342 14.78342 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
For Hydrogen: Wyckoff position b, x = -0.03030, y = -0.42190, z
1 0.96970 0.57810 0.51040
49 0.53030 0.42190 0.01040
33 0.03030 0.07810 0.98960
17 0.46970 0.92190 0.48960
177 0.51040 0.96970 0.57810
145 0.98960 0.03030 0.07810
161 0.48960 0.46970 0.92190
129 0.01040 0.53030 0.42190
81 0.57810 0.51040 0.96970
65 0.92190 0.48960 0.46970
97 0.42190 0.01040 0.53030
113 0.07810 0.98960 0.03030
For Hydrogen: Wyckoff position b, x = -0.09660, y = -0.23680, z

2 0.90340 0.76320 0.48390
50 0.59660 0.23680 0.98390
34 0.09660 0.26320 0.01610
18 0.40340 0.73680 0.51610
178 0.48390 0.90340 0.76320
146 0.01610 0.09660 0.26320
162 0.51610 0.40340 0.73680
130 0.98390 0.59660 0.23680
82 0.76320 0.48390 0.90340
66 0.73680 0.51610 0.40340
98 0.23680 0.98390 0.59660
114 0.26320 0.01610 0.09660
For Hydrogen: Wyckoff position b, x = -0.17400, y = -0.21240, z
3 0.82600 0.78760 0.43740
51 0.67400 0.21240 0.93740
35 0.17400 0.28760 0.06260
19 0.32600 0.71240 0.56260
179 0.43740 0.82600 0.78760
147 0.06260 0.17400 0.28760
163 0.56260 0.32600 0.71240
131 0.93740 0.67400 0.21240
83 0.78760 0.43740 0.82600
67 0.71240 0.56260 0.32600
99 0.21240 0.93740 0.67400
115 0.28760 0.06260 0.17400
For Hydrogen: Wyckoff position b, x = -0.10270, y = -0.19520, z
4 0.89730 0.80480 0.38590
52 0.60270 0.19520 0.88590
36 0.10270 0.30480 0.11410
20 0.39730 0.69520 0.61410
180 0.38590 0.89730 0.80480
148 0.11410 0.10270 0.30480
164 0.61410 0.39730 0.69520
132 0.88590 0.60270 0.19520
84 0.80480 0.38590 0.89730
68 0.69520 0.61410 0.39730
100 0.19520 0.88590 0.60270
116 0.30480 0.11410 0.10270
For Hydrogen: Wyckoff position b, x = 0.22440, y = 0.23320, z
5 0.22440 0.23320 0.67920
53 0.27560 0.76680 0.17920
37 0.77560 0.73320 0.82080
21 0.72440 0.26680 0.32080
181 0.67920 0.22440 0.23320

149 0.82080 0.77560 0.73320
165 0.32080 0.72440 0.26680
133 0.17920 0.27560 0.76680
85 0.23320 0.67920 0.22440
69 0.26680 0.32080 0.72440
101 0.76680 0.17920 0.27560
117 0.73320 0.82080 0.77560
For Hydrogen: Wyckoff position b, x = 0.23870, y = -0.48380, z
6 0.23870 0.51620 0.64950
54 0.26130 0.48380 0.14950
38 0.76130 0.01620 0.85050
22 0.73870 0.98380 0.35050
182 0.64950 0.23870 0.51620
150 0.85050 0.76130 0.01620
166 0.35050 0.73870 0.98380
134 0.14950 0.26130 0.48380
86 0.51620 0.64950 0.23870
70 0.98380 0.35050 0.73870
102 0.48380 0.14950 0.26130
118 0.01620 0.85050 0.76130
For Hydrogen: Wyckoff position b, x = 0.13090, y = -0.44190, z
7 0.13090 0.55810 0.65250
55 0.36910 0.44190 0.15250
39 0.86910 0.05810 0.84750
23 0.63090 0.94190 0.34750
183 0.65250 0.13090 0.55810
151 0.84750 0.86910 0.05810
167 0.34750 0.63090 0.94190
135 0.15250 0.36910 0.44190
87 0.55810 0.65250 0.13090
71 0.94190 0.34750 0.63090
103 0.44190 0.15250 0.36910
119 0.05810 0.84750 0.86910
For Hydrogen: Wyckoff position b, x = 0.17950, y = -0.46950, z
8 0.17950 0.53050 0.55380
56 0.32050 0.46950 0.05380
40 0.82050 0.03050 0.94620
24 0.67950 0.96950 0.44620
184 0.55380 0.17950 0.53050
152 0.94620 0.82050 0.03050
168 0.44620 0.67950 0.96950
136 0.05380 0.32050 0.46950
88 0.53050 0.55380 0.17950
72 0.96950 0.44620 0.67950

104 0.46950 0.05380 0.32050
120 0.03050 0.94620 0.82050
For Hydrogen: Wyckoff position b, x = 0.42300, y = -0.01230, z
9 0.42300 0.98770 0.97400
57 0.07700 0.01230 0.47400
41 0.57700 0.48770 0.52600
25 0.92300 0.51230 0.02600
185 0.97400 0.42300 0.98770
153 0.52600 0.57700 0.48770
169 0.02600 0.92300 0.51230
137 0.47400 0.07700 0.01230
89 0.98770 0.97400 0.42300
73 0.51230 0.02600 0.92300
105 0.01230 0.47400 0.07700
121 0.48770 0.52600 0.57700
For Hydrogen: Wyckoff position b, x = 0.48140, y = 0.08890, z
10 0.48140 0.08890 0.73470
58 0.01860 0.91110 0.23470
42 0.51860 0.58890 0.76530
26 0.98140 0.41110 0.26530
186 0.73470 0.48140 0.08890
154 0.76530 0.51860 0.58890
170 0.26530 0.98140 0.41110
138 0.23470 0.01860 0.91110
90 0.08890 0.73470 0.48140
74 0.41110 0.26530 0.98140
106 0.91110 0.23470 0.01860
122 0.58890 0.76530 0.51860
For Hydrogen: Wyckoff position b, x = 0.41350, y = 0.15840, z
11 0.41350 0.15840 0.70530
59 0.08650 0.84160 0.20530
43 0.58650 0.65840 0.79470
27 0.91350 0.34160 0.29470
187 0.70530 0.41350 0.15840
155 0.79470 0.58650 0.65840
171 0.29470 0.91350 0.34160
139 0.20530 0.08650 0.84160
91 0.15840 0.70530 0.41350
75 0.34160 0.29470 0.91350
107 0.84160 0.20530 0.08650
123 0.65840 0.79470 0.58650
For Hydrogen: Wyckoff position b, x = 0.37780, y = 0.06870, z
12 0.37780 0.06870 0.70720
60 0.12220 0.93130 0.20720

44 0.62220 0.56870 0.79280
28 0.87780 0.43130 0.29280
188 0.70720 0.37780 0.06870
156 0.79280 0.62220 0.56870
172 0.29280 0.87780 0.43130
140 0.20720 0.12220 0.93130
92 0.06870 0.70720 0.37780
76 0.43130 0.29280 0.87780
108 0.93130 0.20720 0.12220
124 0.56870 0.79280 0.62220
For Hydrogen: Wyckoff position b, x = -0.31970, y = -0.23200, z
13 0.68030 0.76800 0.26620
61 0.81970 0.23200 0.76620
45 0.31970 0.26800 0.23380
29 0.18030 0.73200 0.73380
189 0.26620 0.68030 0.76800
157 0.23380 0.31970 0.26800
173 0.73380 0.18030 0.73200
141 0.76620 0.81970 0.23200
93 0.76800 0.26620 0.68030
77 0.73200 0.73380 0.18030
109 0.23200 0.76620 0.81970
125 0.26800 0.23380 0.31970
For Hydrogen: Wyckoff position b, x = -0.43080, y = -0.16940, z
14 0.56920 0.83060 0.96390
62 0.93080 0.16940 0.46390
46 0.43080 0.33060 0.53610
30 0.06920 0.66940 0.03610
190 0.96390 0.56920 0.83060
158 0.53610 0.43080 0.33060
174 0.03610 0.06920 0.66940
142 0.46390 0.93080 0.16940
94 0.83060 0.96390 0.56920
78 0.66940 0.03610 0.06920
110 0.16940 0.46390 0.93080
126 0.33060 0.53610 0.43080
For Hydrogen: Wyckoff position b, x = -0.33650, y = -0.24010, z
15 0.66350 0.75990 0.98810
63 0.83650 0.24010 0.48810
47 0.33650 0.25990 0.51190
31 0.16350 0.74010 0.01190
191 0.98810 0.66350 0.75990
159 0.51190 0.33650 0.25990
175 0.01190 0.16350 0.74010

143 0.48810 0.83650 0.24010
95 0.75990 0.98810 0.66350
79 0.74010 0.01190 0.16350
111 0.24010 0.48810 0.83650
127 0.25990 0.51190 0.33650
For Hydrogen: Wyckoff position b, x = -0.32410, y = -0.13650, z
16 0.67590 0.86350 0.95450
64 0.82410 0.13650 0.45450
48 0.32410 0.36350 0.54550
32 0.17590 0.63650 0.04550
192 0.95450 0.67590 0.86350
160 0.54550 0.32410 0.36350
176 0.04550 0.17590 0.63650
144 0.45450 0.82410 0.13650
96 0.86350 0.95450 0.67590
80 0.63650 0.04550 0.17590
112 0.13650 0.45450 0.82410
128 0.36350 0.54550 0.32410
For Lithium: Wyckoff position a, x = 0.11860
193 0.88140 0.61860 0.38140
205 0.61860 0.38140 0.88140
201 0.11860 0.11860 0.11860
197 0.38140 0.88140 0.61860
For Lithium: Wyckoff position a, x = -0.12470
194 0.12470 0.37530 0.62470
206 0.37530 0.62470 0.12470
202 0.87530 0.87530 0.87530
198 0.62470 0.12470 0.37530
For Lithium: Wyckoff position a, x = -0.37640
195 0.37640 0.12360 0.87640
207 0.12360 0.87640 0.37640
203 0.62360 0.62360 0.62360
199 0.87640 0.37640 0.12360
For Lithium: Wyckoff position a, x = 0.38140
196 0.61860 0.88140 0.11860
208 0.88140 0.11860 0.61860
204 0.38140 0.38140 0.38140
200 0.11860 0.61860 0.88140
For Nitrogen: Wyckoff position b, x = -0.12600, y = -0.24250, z
209 0.87400 0.75750 0.42530
221 0.62600 0.24250 0.92530
217 0.12600 0.25750 0.07470
213 0.37400 0.74250 0.57470
253 0.42530 0.87400 0.75750

245 0.07470 0.12600 0.25750
249 0.57470 0.37400 0.74250
241 0.92530 0.62600 0.24250
229 0.75750 0.42530 0.87400
225 0.74250 0.57470 0.37400
233 0.24250 0.92530 0.62600
237 0.25750 0.07470 0.12600
For Nitrogen: Wyckoff position b, x = 0.17390, y = -0.49260, z
210 0.17390 0.50740 0.62220
222 0.32610 0.49260 0.12220
218 0.82610 0.00740 0.87780
214 0.67390 0.99260 0.37780
254 0.62220 0.17390 0.50740
246 0.87780 0.82610 0.00740
250 0.37780 0.67390 0.99260
242 0.12220 0.32610 0.49260
230 0.50740 0.62220 0.17390
226 0.99260 0.37780 0.67390
234 0.49260 0.12220 0.32610
238 0.00740 0.87780 0.82610
For Nitrogen: Wyckoff position b, x = 0.41570, y = 0.10730, z
211 0.41570 0.10730 0.74430
223 0.08430 0.89270 0.24430
219 0.58430 0.60730 0.75570
215 0.91570 0.39270 0.25570
255 0.74430 0.41570 0.10730
247 0.75570 0.58430 0.60730
251 0.25570 0.91570 0.39270
243 0.24430 0.08430 0.89270
231 0.10730 0.74430 0.41570
227 0.39270 0.25570 0.91570
235 0.89270 0.24430 0.08430
239 0.60730 0.75570 0.58430
For Nitrogen: Wyckoff position b, x = -0.36560, y = -0.17210, z
212 0.63440 0.82790 0.99470
224 0.86560 0.17210 0.49470
220 0.36560 0.32790 0.50530
216 0.13440 0.67210 0.00530
256 0.99470 0.63440 0.82790
248 0.50530 0.36560 0.32790
252 0.00530 0.13440 0.67210
244 0.49470 0.86560 0.17210
232 0.82790 0.99470 0.63440
228 0.67210 0.00530 0.13440

236 0.17210 0.49470 0.86560
240 0.32790 0.50530 0.36560
For Nitrogen: Wyckoff position a, x = 0.04550
257 0.95450 0.54550 0.45450
269 0.54550 0.45450 0.95450
265 0.04550 0.04550 0.04550
261 0.45450 0.95450 0.54550
For Nitrogen: Wyckoff position a, x = -0.20620
258 0.20620 0.29380 0.70620
270 0.29380 0.70620 0.20620
266 0.79380 0.79380 0.79380
262 0.70620 0.20620 0.29380
For Nitrogen: Wyckoff position a, x = -0.45770
259 0.45770 0.04230 0.95770
271 0.04230 0.95770 0.45770
267 0.54230 0.54230 0.54230
263 0.95770 0.45770 0.04230
For Nitrogen: Wyckoff position a, x = 0.29280
260 0.70720 0.79280 0.20720
272 0.79280 0.20720 0.70720
268 0.29280 0.29280 0.29280
264 0.20720 0.70720 0.79280

2.10 1-Dimensional Chain

0 GPa, Enthalpy: -81.374893 eV
$a, b, c, \alpha, \beta, \gamma$: 19.96223 19.96223 6.02273 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
Wyckoff position o, x = 0.09179, y = 0.03380, z
1 0.09179 0.03380 0.30106
4 0.09179 0.96620 0.69894
12 0.90821 0.03380 0.69894
8 0.90821 0.96620 0.30106
3 0.03380 0.09179 0.30106
6 0.03380 0.90821 0.69894
11 0.96620 0.09179 0.69894
7 0.96620 0.90821 0.30106
Wyckoff position n, x = 0.09219, z = 0.10886
2 0.09219 0.09219 0.10886
5 0.09219 0.90781 0.89114
10 0.90781 0.09219 0.89114
9 0.90781 0.90781 0.10886
Wyckoff position a

13 0.00000 0.00000 0.00000
Wyckoff position n, x = 0.06110, z = 0.19785
14 0.06110 0.06110 0.19785
15 0.06110 0.93890 0.80215
17 0.93890 0.06110 0.80215
16 0.93890 0.93890 0.19785

2.11 2-Dimensional Sheet

0 GPa, Enthalpy: -81.557768 eV
$a, b, c, \alpha, \beta, \gamma$: 6.13410 6.13410 19.13512 90.00000 90.00000 90.00000
Atomic positions in terms of a,b,c:
Wyckoff position o, x = 0.10885, y = -0.29783, z
1 0.10885 0.70217 0.90309
12 0.10885 0.29783 0.09691
8 0.89115 0.70217 0.09691
4 0.89115 0.29783 0.90309
5 0.70217 0.10885 0.90309
9 0.70217 0.89115 0.09691
10 0.29783 0.10885 0.09691
2 0.29783 0.89115 0.90309
Wyckoff position n, x = 0.30003, z = 0.03730
3 0.30003 0.69997 0.96270
11 0.30003 0.30003 0.03730
7 0.69997 0.69997 0.03730
6 0.69997 0.30003 0.96270
Wyckoff position a
13 0.00000 0.00000 0.00000
Wyckoff position n, x = 0.19750, z = 0.06453
14 0.19750 0.80250 0.93547
17 0.19750 0.19750 0.06453
16 0.80250 0.80250 0.06453
15 0.80250 0.19750 0.93547

References

[1] Young, V. G.; Glaunsinger, W. S.; Von Dreele, R. B. *J. Am. Chem. Soc.* **1989**, *111*, 9260–9261.

[2] Ibberson, R. M.; Fowkes, A. J.; Rosseinsky, M. J.; David, W. I. F.; Edwards, P. P. *Angew. Chem. Int. Ed.* **2009**, *48*, 1435–1438.