Result for pseudosymmetry search

Formulae

Input of the program

Initial structure:

```
146
14.0618 14.0618 9.8513 90.0 90.0 119.99999999999999
18
Ba       1        3a       0.333334        0.666667        0.140761
Mn       2        3a       0.333334        0.666667        0.741352
H        3        9b       0.132631        0.287676        0.247315
H        4        9b       0.138290        0.352371        0.089110
H        5        9b       0.040283        0.554809        0.350041
H        6        9b       0.948752        0.490121        0.210844
H        7        9b       0.995815        0.345257        0.249007
H        8        9b       0.101635        0.426656        0.368788
H        9        9b       0.345995        0.418999        0.063668
H        10       9b       0.313100        0.327490        0.203755
C        11       9b       0.153210        0.366360        0.199175
C        12       9b       0.035075        0.547873        0.238428
C        13       9b       0.083152        0.408520        0.259759
C        14       9b       0.341810        0.413513        0.175383
Br       15       9b       0.515291        0.757896        0.858808
Br       16       3a       0.333334        0.666667        0.491818
O        17       9b       0.105031        0.507492        0.190317
O        18       9b       0.266482        0.447005        0.223750
```

Maximum tolerance: 4

Grid: 0.4 Angstroms

Summary search results

Pseudosymmetry search among minimal supergroups.

Case #	Supergroup G	Index i	Index i_k	(P,p)	Tr. Matrix	Δ_{max}	u_{max}
1	*R*-3 (148)	2	1	**a,b,c** ; 0,0,0	[1 0 0] [0] [0 1 0] [0] [0 0 1] [0]	3.0832	1.5416

Idealized structures

1# Supergroup *R*-3 (148): a,b,c ; 0,0,0 and index 2

Displacements:

Atom	Idealized Coordinates	u_x	u_y	u_z	|u|
Ba1	(0.3333, 0.6667, 0.6667)	0.000000	0.000000	-0.109239	1.0761
Mn2	(0.3333, 0.6667, 0.1667)	0.000000	0.000000	-0.008648	0.0852
H3	(0.1290, 0.2849, 0.6849)	0.003667	0.002795	-0.020920	0.2113
H4	(0.1452, 0.3630, 0.5362)	-0.006926	-0.010622	-0.030424	0.3272
H5	(0.0297, 0.5511, 0.7971)	0.010623	0.003697	-0.030424	0.3272
H6	(0.9515, 0.4892, 0.6484)	-0.002795	0.000871	-0.020920	0.2113
H7	(0.9950, 0.3465, 0.6893)	0.000829	-0.001233	-0.023619	0.2340
H8	(0.0936, 0.4165, 0.8192)	0.007985	0.010160	-0.033772	0.3573
H9	(0.3438, 0.4270, 0.5141)	0.002174	-0.007985	-0.033772	0.3573
H10	(0.3152, 0.3283, 0.6440)	-0.002063	-0.000830	-0.023619	0.2340
C11	(0.1535, 0.3674, 0.6470)	-0.000329	-0.001025	-0.031198	0.3076
C12	(0.0341, 0.5472, 0.6863)	0.001024	0.000695	-0.031198	0.3076
C13	(0.0817, 0.4068, 0.7089)	0.001486	0.001742	-0.032428	0.3203
C14	(0.3416, 0.4150, 0.6245)	0.000255	-0.001486	-0.032429	0.3203
Br15	(0.4243, 0.7123, 0.3502)	0.090979	0.045615	-0.074687	1.3300
Br16	(0.3787, 0.7576, 0.9832)	-0.045364	-0.090979	-0.074687	1.3300
O17	(0.1094, 0.5107, 0.6499)	-0.004320	-0.003182	-0.042966	0.4268
O18	(0.2653, 0.4427, 0.6834)	0.001138	0.004320	-0.042966	0.4268

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute displacement given in Å

Optimized polar structure:

```
# Origin shifted with t = (0.000000, 0.000000, 0.416667)
146
14.0618 14.0618 9.8513 90.00 90.00 120.00
18
Ba      1       -       0.333334        0.666667        0.557428
Mn      2       -       0.333334        0.666667        0.158019
H       3       -       0.132631        0.287676        0.663982
H       4       -       0.138290        0.352371        0.505777
H       5       -       0.040283        0.554809        0.766708
H       6       -       0.948752        0.490121        0.627511
H       7       -       0.995815        0.345257        0.665674
H       8       -       0.101635        0.426656        0.785455
H       9       -       0.345995        0.418999        0.480335
H       10      -       0.313100        0.327490        0.620422
C       11      -       0.153210        0.366360        0.615842
C       12      -       0.035075        0.547873        0.655095
C       13      -       0.083152        0.408520        0.676426
C       14      -       0.341810        0.413513        0.592050
Br      15      -       0.515291        0.757896        0.275475
Br      16      -       0.333334        0.666667        0.908485
```

```
O       17      -       0.105031        0.507492        0.606984
O       18      -       0.266482        0.447005        0.640417
```

Idealized structure (subgroup setting):

```
146
14.0618 14.0618 9.8513 90.00 90.00 120.00
18
Ba      1       3a      0.333333        0.666667        0.666667
Mn      2       3a      0.333333        0.666667        0.166667
H       3       9b      0.128964        0.284881        0.684902
H       4       9b      0.145216        0.362993        0.536201
H       5       9b      0.029660        0.551112        0.797132
H       6       9b      0.951547        0.489250        0.648431
H       7       9b      0.994986        0.346490        0.689293
H       8       9b      0.093650        0.416496        0.819227
H       9       9b      0.343821        0.426984        0.514107
H       10      9b      0.315163        0.328320        0.644041
C       11      9b      0.153539        0.367385        0.647040
C       12      9b      0.034051        0.547178        0.686293
C       13      9b      0.081666        0.406778        0.708854
C       14      9b      0.341555        0.414999        0.624479
Br      15      9b      0.424312        0.712281        0.350162
Br      16      9b      0.378698        0.757646        0.983172
O       17      9b      0.109351        0.510674        0.649950
O       18      9b      0.265344        0.442685        0.683383
```

Idealized structure (supergroup setting):

```
148
14.0618 14.0618 9.8513 90.00 90.00 120.00
10
Ba      1       3a      0.333333        0.666667        0.666667
Mn      2       3b      0.333333        0.666667        0.166667
H       3       18f     0.128964        0.284881        0.684902
H       4       18f     0.145216        0.362993        0.536201
H       8       18f     0.093650        0.416496        0.819227
H       10      18f     0.315163        0.328320        0.644041
C       11      18f     0.153539        0.367385        0.647040
C       13      18f     0.081666        0.406778        0.708854
Br      15      18f     0.424312        0.712281        0.350162
O       17      18f     0.109351        0.510674        0.649950
```

Notes:

- Idealized structure with space group 148 related with the given by the transformation **a,b,c** ; 0,0,0 and index 2
- Cell parameters have not been symmetrized. They may include in general some symmetry breaking strain, to be removed by hand.
- Some problems might be present in the assignment of Wyckoff positions of the idealized orbits due to the decimal point errors.

Continue to search for pseudosymmetry with this structure (#148) | Visualize this structure | CIF File

Plot the progress so far

WARNING: The splittings of the Wyckoff positions of the idealized atoms do not correspond to those of the initial structure.

[Click here to hide full report]

Pseudosymmetry search full report

1# Supergroup *R*-3 (148): a,b,c ; 0,0,0 and index 2

Transformation matrix: a,b,c ; 0,0,0 (index = 2)

```
[      1      0      0 ] [       0]
[      0      1      0 ] [       0]
[      0      0      1 ] [       t]
```

Coset representative: -x,-y,-z

Maximum distance: 3.0832

Pairings and distances:

Atom in S	Coordinates in S	Atom in gS	Δ_x	Δ_y	Δ_z	|Δ|
Ba1[1]	(0.333334,0.666667,0.557428)	Ba1[3]	0.0000	0.0000	-0.2185	2.1523
Ba1[2]	(0.000000,0.000000,0.890762)	Ba1[2]	0.0000	0.0000	-0.2185	2.1523
Ba1[3]	(0.666667,0.333333,0.224095)	Ba1[1]	0.0000	0.0000	-0.2185	2.1523
Mn2[1]	(0.333334,0.666667,0.158019)	Mn2[3]	0.0000	0.0000	-0.0173	0.1704
Mn2[2]	(0.000000,0.000000,0.491353)	Mn2[2]	0.0000	0.0000	-0.0173	0.1704
Mn2[3]	(0.666667,0.333333,0.824686)	Mn2[1]	0.0000	0.0000	-0.0173	0.1704
H3[1]	(0.132631,0.287676,0.663982)	H6[9]	0.0073	0.0056	-0.0418	0.4226
H3[2]	(0.712324,0.844955,0.663982)	H6[7]	-0.0056	0.0017	-0.0418	0.4226
H3[3]	(0.155045,0.867369,0.663982)	H6[8]	-0.0017	-0.0073	-0.0418	0.4226
H3[4]	(0.799298,0.621010,0.997316)	H6[6]	0.0073	0.0056	-0.0418	0.4226
H3[5]	(0.378990,0.178288,0.997316)	H6[4]	-0.0056	0.0017	-0.0418	0.4226
H3[6]	(0.821712,0.200702,0.997316)	H6[5]	-0.0017	-0.0073	-0.0418	0.4226
H3[7]	(0.465964,0.954343,0.330649)	H6[3]	0.0073	0.0056	-0.0418	0.4226
H3[8]	(0.045657,0.511621,0.330649)	H6[1]	-0.0056	0.0017	-0.0418	0.4226
H3[9]	(0.488379,0.534036,0.330649)	H6[2]	-0.0017	-0.0073	-0.0418	0.4226
H4[1]	(0.138290,0.352371,0.505777)	H5[9]	-0.0139	-0.0212	-0.0608	0.6545
H4[2]	(0.647629,0.785919,0.505777)	H5[7]	0.0212	0.0074	-0.0608	0.6545
H4[3]	(0.214081,0.861710,0.505777)	H5[8]	-0.0074	0.0139	-0.0608	0.6545
H4[4]	(0.804957,0.685704,0.839110)	H5[6]	-0.0138	-0.0212	-0.0608	0.6545
H4[5]	(0.314296,0.119253,0.839110)	H5[4]	0.0212	0.0074	-0.0608	0.6545
H4[6]	(0.880747,0.195043,0.839110)	H5[5]	-0.0074	0.0138	-0.0608	0.6545
H4[7]	(0.471623,0.019037,0.172444)	H5[3]	-0.0139	-0.0212	-0.0608	0.6545
H4[8]	(0.980963,0.452586,0.172444)	H5[1]	0.0212	0.0074	-0.0608	0.6545
H4[9]	(0.547414,0.528377,0.172444)	H5[2]	-0.0074	0.0139	-0.0608	0.6545
H5[1]	(0.040283,0.554809,0.766708)	H4[8]	0.0212	0.0074	-0.0608	0.6545
H5[2]	(0.445191,0.485474,0.766708)	H4[9]	-0.0074	0.0139	-0.0608	0.6545
H5[3]	(0.514526,0.959717,0.766708)	H4[7]	-0.0139	-0.0212	-0.0608	0.6545

H5[4]	(0.706950,0.888142,0.100041)	H4[5]	0.0212	0.0074	-0.0608	0.6545
H5[5]	(0.111858,0.818807,0.100041)	H4[6]	-0.0074	0.0138	-0.0608	0.6545
H5[6]	(0.181193,0.293050,0.100041)	H4[4]	-0.0138	-0.0212	-0.0608	0.6545
H5[7]	(0.373616,0.221476,0.433375)	H4[2]	0.0212	0.0074	-0.0608	0.6545
H5[8]	(0.778524,0.152141,0.433375)	H4[3]	-0.0074	0.0139	-0.0608	0.6545
H5[9]	(0.847859,0.626384,0.433375)	H4[1]	-0.0139	-0.0212	-0.0608	0.6545
H6[1]	(0.948752,0.490121,0.627511)	H3[8]	-0.0056	0.0017	-0.0418	0.4226
H6[2]	(0.509879,0.458631,0.627511)	H3[9]	-0.0017	-0.0073	-0.0418	0.4226
H6[3]	(0.541369,0.051248,0.627511)	H3[7]	0.0073	0.0056	-0.0418	0.4226
H6[4]	(0.615419,0.823454,0.960845)	H3[5]	-0.0056	0.0017	-0.0418	0.4226
H6[5]	(0.176546,0.791964,0.960845)	H3[6]	-0.0017	-0.0073	-0.0418	0.4226
H6[6]	(0.208036,0.384581,0.960845)	H3[4]	0.0073	0.0056	-0.0418	0.4226
H6[7]	(0.282085,0.156788,0.294178)	H3[2]	-0.0056	0.0017	-0.0418	0.4226
H6[8]	(0.843212,0.125298,0.294178)	H3[3]	-0.0017	-0.0073	-0.0418	0.4226
H6[9]	(0.874702,0.717915,0.294178)	H3[1]	0.0073	0.0056	-0.0418	0.4226
H7[1]	(0.995815,0.345257,0.665674)	H10[8]	0.0017	-0.0025	-0.0472	0.4681
H7[2]	(0.654743,0.650558,0.665674)	H10[9]	0.0025	0.0041	-0.0472	0.4681
H7[3]	(0.349442,0.004185,0.665674)	H10[7]	-0.0041	-0.0017	-0.0472	0.4681
H7[4]	(0.662482,0.678591,0.999007)	H10[5]	0.0017	-0.0025	-0.0472	0.4681
H7[5]	(0.321409,0.983891,0.999007)	H10[6]	0.0025	0.0041	-0.0472	0.4681
H7[6]	(0.016109,0.337518,0.999007)	H10[4]	-0.0041	-0.0017	-0.0472	0.4681
H7[7]	(0.329149,0.011924,0.332340)	H10[2]	0.0017	-0.0025	-0.0472	0.4681
H7[8]	(0.988076,0.317225,0.332340)	H10[3]	0.0025	0.0041	-0.0472	0.4681
H7[9]	(0.682775,0.670851,0.332340)	H10[1]	-0.0041	-0.0017	-0.0472	0.4681
H8[1]	(0.101635,0.426656,0.785455)	H9[8]	0.0160	0.0203	-0.0675	0.7146
H8[2]	(0.573344,0.674979,0.785455)	H9[9]	-0.0203	-0.0043	-0.0675	0.7146
H8[3]	(0.325021,0.898365,0.785455)	H9[7]	0.0043	-0.0160	-0.0675	0.7146
H8[4]	(0.768302,0.759989,0.118788)	H9[5]	0.0160	0.0203	-0.0675	0.7146
H8[5]	(0.240011,0.008313,0.118788)	H9[6]	-0.0203	-0.0043	-0.0675	0.7146
H8[6]	(0.991687,0.231698,0.118788)	H9[4]	0.0043	-0.0160	-0.0675	0.7146
H8[7]	(0.434969,0.093323,0.452122)	H9[2]	0.0160	0.0203	-0.0675	0.7146
H8[8]	(0.906677,0.341646,0.452122)	H9[3]	-0.0203	-0.0043	-0.0675	0.7146
H8[9]	(0.658354,0.565031,0.452122)	H9[1]	0.0043	-0.0160	-0.0675	0.7146
H9[1]	(0.345995,0.418999,0.480335)	H8[9]	0.0043	-0.0160	-0.0675	0.7146
H9[2]	(0.581001,0.926996,0.480335)	H8[7]	0.0160	0.0203	-0.0675	0.7146
H9[3]	(0.073004,0.654005,0.480335)	H8[8]	-0.0203	-0.0043	-0.0675	0.7146

H9[4]	(0.012661,0.752332,0.813669)	H8[6]	0.0043	-0.0160	-0.0675	0.7146
H9[5]	(0.247668,0.260329,0.813669)	H8[4]	0.0160	0.0203	-0.0675	0.7146
H9[6]	(0.739671,0.987339,0.813669)	H8[5]	-0.0203	-0.0043	-0.0675	0.7146
H9[7]	(0.679328,0.085666,0.147002)	H8[3]	0.0043	-0.0160	-0.0675	0.7146
H9[8]	(0.914335,0.593663,0.147002)	H8[1]	0.0160	0.0203	-0.0675	0.7146
H9[9]	(0.406337,0.320672,0.147002)	H8[2]	-0.0203	-0.0043	-0.0675	0.7146
H10[1]	(0.313100,0.327490,0.620422)	H7[9]	-0.0041	-0.0017	-0.0472	0.4681
H10[2]	(0.672510,0.985610,0.620422)	H7[7]	0.0017	-0.0025	-0.0472	0.4681
H10[3]	(0.014390,0.686900,0.620422)	H7[8]	0.0025	0.0041	-0.0472	0.4681
H10[4]	(0.979767,0.660824,0.953755)	H7[6]	-0.0041	-0.0017	-0.0472	0.4681
H10[5]	(0.339176,0.318943,0.953755)	H7[4]	0.0017	-0.0025	-0.0472	0.4681
H10[6]	(0.681057,0.020233,0.953755)	H7[5]	0.0025	0.0041	-0.0472	0.4681
H10[7]	(0.646434,0.994157,0.287089)	H7[3]	-0.0041	-0.0017	-0.0472	0.4681
H10[8]	(0.005843,0.652277,0.287089)	H7[1]	0.0017	-0.0025	-0.0472	0.4681
H10[9]	(0.347723,0.353566,0.287089)	H7[2]	0.0025	0.0041	-0.0472	0.4681
C11[1]	(0.153210,0.366360,0.615842)	C12[9]	-0.0007	-0.0020	-0.0624	0.6152
C11[2]	(0.633640,0.786850,0.615842)	C12[7]	0.0020	0.0014	-0.0624	0.6152
C11[3]	(0.213150,0.846790,0.615842)	C12[8]	-0.0014	0.0007	-0.0624	0.6152
C11[4]	(0.819877,0.699694,0.949175)	C12[6]	-0.0007	-0.0020	-0.0624	0.6152
C11[5]	(0.300306,0.120183,0.949175)	C12[4]	0.0020	0.0014	-0.0624	0.6152
C11[6]	(0.879817,0.180123,0.949175)	C12[5]	-0.0014	0.0007	-0.0624	0.6152
C11[7]	(0.486544,0.033027,0.282509)	C12[3]	-0.0007	-0.0020	-0.0624	0.6152
C11[8]	(0.966973,0.453516,0.282509)	C12[1]	0.0020	0.0014	-0.0624	0.6152
C11[9]	(0.546484,0.513456,0.282509)	C12[2]	-0.0014	0.0007	-0.0624	0.6152
C12[1]	(0.035075,0.547873,0.655095)	C11[8]	0.0020	0.0014	-0.0624	0.6152
C12[2]	(0.452127,0.487202,0.655095)	C11[9]	-0.0014	0.0007	-0.0624	0.6152
C12[3]	(0.512798,0.964925,0.655095)	C11[7]	-0.0007	-0.0020	-0.0624	0.6152
C12[4]	(0.701742,0.881206,0.988429)	C11[5]	0.0020	0.0014	-0.0624	0.6152
C12[5]	(0.118794,0.820536,0.988429)	C11[6]	-0.0014	0.0007	-0.0624	0.6152
C12[6]	(0.179464,0.298258,0.988429)	C11[4]	-0.0007	-0.0020	-0.0624	0.6152
C12[7]	(0.368409,0.214540,0.321762)	C11[2]	0.0020	0.0014	-0.0624	0.6152
C12[8]	(0.785460,0.153869,0.321762)	C11[3]	-0.0014	0.0007	-0.0624	0.6152
C12[9]	(0.846131,0.631591,0.321762)	C11[1]	-0.0007	-0.0020	-0.0624	0.6152
C13[1]	(0.083152,0.408520,0.676426)	C14[8]	0.0030	0.0035	-0.0649	0.6406
C13[2]	(0.591480,0.674633,0.676426)	C14[9]	-0.0035	-0.0005	-0.0649	0.6406
C13[3]	(0.325367,0.916848,0.676426)	C14[7]	0.0005	-0.0030	-0.0649	0.6406

C13[4]	(0.749819,0.741853,0.009759)	C14[5]	0.0030	0.0035	-0.0649	0.6406
C13[5]	(0.258147,0.007966,0.009759)	C14[6]	-0.0035	-0.0005	-0.0649	0.6406
C13[6]	(0.992034,0.250181,0.009759)	C14[4]	0.0005	-0.0030	-0.0649	0.6406
C13[7]	(0.416486,0.075186,0.343092)	C14[2]	0.0030	0.0035	-0.0649	0.6406
C13[8]	(0.924814,0.341299,0.343092)	C14[3]	-0.0035	-0.0005	-0.0649	0.6406
C13[9]	(0.658701,0.583514,0.343092)	C14[1]	0.0005	-0.0030	-0.0649	0.6406
C14[1]	(0.341810,0.413513,0.592050)	C13[9]	0.0005	-0.0030	-0.0649	0.6406
C14[2]	(0.586487,0.928297,0.592050)	C13[7]	0.0030	0.0035	-0.0649	0.6406
C14[3]	(0.071703,0.658190,0.592050)	C13[8]	-0.0035	-0.0005	-0.0649	0.6406
C14[4]	(0.008477,0.746847,0.925384)	C13[6]	0.0005	-0.0030	-0.0649	0.6406
C14[5]	(0.253154,0.261630,0.925384)	C13[4]	0.0030	0.0035	-0.0649	0.6406
C14[6]	(0.738370,0.991523,0.925384)	C13[5]	-0.0035	-0.0005	-0.0649	0.6406
C14[7]	(0.675143,0.080180,0.258717)	C13[3]	0.0005	-0.0030	-0.0649	0.6406
C14[8]	(0.919820,0.594964,0.258717)	C13[1]	0.0030	0.0035	-0.0649	0.6406
C14[9]	(0.405037,0.324857,0.258717)	C13[2]	-0.0035	-0.0005	-0.0649	0.6406
Br15[1]	(0.515291,0.757896,0.275475)	Br16[3]	0.1820	0.0912	-0.1494	2.6600
Br15[2]	(0.242104,0.757395,0.275475)	Br15[7]	0.0907	0.1820	0.2176	3.0832
Br15[3]	(0.242605,0.484709,0.275475)	Br15[8]	-0.1820	-0.0912	0.2176	3.0832
Br15[4]	(0.181958,0.091229,0.608808)	Br16[2]	0.1820	0.0912	-0.1494	2.6600
Br15[5]	(0.908771,0.090729,0.608808)	Br15[4]	0.0907	0.1820	0.2176	3.0832
Br15[6]	(0.909271,0.818042,0.608808)	Br15[5]	-0.1820	-0.0912	0.2176	3.0832
Br15[7]	(0.848624,0.424562,0.942141)	Br16[1]	0.1820	0.0912	-0.1494	2.6600
Br15[8]	(0.575438,0.424062,0.942141)	Br15[1]	0.0907	0.1820	0.2176	3.0832
Br15[9]	(0.575938,0.151376,0.942141)	Br15[2]	-0.1820	-0.0912	0.2176	3.0832
Br16[1]	(0.333334,0.666667,0.908485)	Br15[9]	-0.0907	-0.1820	-0.1494	2.6600
Br16[2]	(0.000000,0.000000,0.241818)	Br15[6]	-0.0907	-0.1820	-0.1494	2.6600
Br16[3]	(0.666667,0.333333,0.575152)	Br15[3]	-0.0907	-0.1820	-0.1494	2.6600
O17[1]	(0.105031,0.507492,0.606984)	O18[8]	-0.0086	-0.0064	-0.0859	0.8535
O17[2]	(0.492508,0.597539,0.606984)	O18[9]	0.0064	-0.0023	-0.0859	0.8535
O17[3]	(0.402461,0.894969,0.606984)	O18[7]	0.0023	0.0086	-0.0859	0.8535
O17[4]	(0.771698,0.840825,0.940317)	O18[5]	-0.0086	-0.0064	-0.0859	0.8535
O17[5]	(0.159175,0.930872,0.940317)	O18[6]	0.0064	-0.0023	-0.0859	0.8536
O17[6]	(0.069128,0.228302,0.940317)	O18[4]	0.0023	0.0086	-0.0859	0.8535
O17[7]	(0.438364,0.174159,0.273651)	O18[2]	-0.0086	-0.0064	-0.0859	0.8535
O17[8]	(0.825841,0.264206,0.273651)	O18[3]	0.0064	-0.0023	-0.0859	0.8535
O17[9]	(0.735794,0.561636,0.273651)	O18[1]	0.0023	0.0086	-0.0859	0.8535

O18[1]	(0.266482,0.447005,0.640417)	O17[9]	0.0023	0.0086	-0.0859	0.8535
O18[2]	(0.552995,0.819477,0.640417)	O17[7]	-0.0086	-0.0064	-0.0859	0.8535
O18[3]	(0.180523,0.733518,0.640417)	O17[8]	0.0064	-0.0023	-0.0859	0.8535
O18[4]	(0.933149,0.780338,0.973750)	O17[6]	0.0023	0.0086	-0.0859	0.8535
O18[5]	(0.219662,0.152810,0.973750)	O17[4]	-0.0086	-0.0064	-0.0859	0.8535
O18[6]	(0.847190,0.066851,0.973750)	O17[5]	0.0064	-0.0023	-0.0859	0.8536
O18[7]	(0.599815,0.113672,0.307084)	O17[3]	0.0023	0.0086	-0.0859	0.8535
O18[8]	(0.886328,0.486144,0.307084)	O17[1]	-0.0086	-0.0064	-0.0859	0.8535
O18[9]	(0.513856,0.400185,0.307084)	O17[2]	0.0064	-0.0023	-0.0859	0.8535

NOTE: Δ_x, Δ_y and &Delta$_z$ are given in relative units. |Δ| is the absolute distance given in Å

Displacements:

Atom	Idealized Coordinates	u_x	u_y	u_z	|u|
Ba1[1]	(0.3333, 0.6667, 0.6667)	0.000000	0.000000	-0.109239	1.0761
Ba1[2]	(0.0000, 0.0000, 0.0000)	0.000000	0.000000	-0.109238	1.0761
Ba1[3]	(0.6667, 0.3333, 0.3333)	0.000000	0.000000	-0.109239	1.0761
Mn2[1]	(0.3333, 0.6667, 0.1667)	0.000000	0.000000	-0.008648	0.0852
Mn2[2]	(0.0000, 0.0000, 0.5000)	0.000000	0.000000	-0.008647	0.0852
Mn2[3]	(0.6667, 0.3333, 0.8333)	0.000000	0.000000	-0.008648	0.0852
H3[1]	(0.1290, 0.2849, 0.6849)	0.003667	0.002795	-0.020920	0.2113
H3[2]	(0.7151, 0.8441, 0.6849)	-0.002795	0.000871	-0.020920	0.2113
H3[3]	(0.1559, 0.8710, 0.6849)	-0.000871	-0.003667	-0.020920	0.2113
H3[4]	(0.7956, 0.6182, 0.0182)	0.003667	0.002795	-0.020920	0.2113
H3[5]	(0.3818, 0.1774, 0.0182)	-0.002795	0.000871	-0.020920	0.2113
H3[6]	(0.8226, 0.2044, 0.0182)	-0.000871	-0.003667	-0.020920	0.2113
H3[7]	(0.4623, 0.9515, 0.3516)	0.003667	0.002795	-0.020920	0.2113
H3[8]	(0.0485, 0.5108, 0.3516)	-0.002795	0.000871	-0.020920	0.2113
H3[9]	(0.4893, 0.5377, 0.3516)	-0.000871	-0.003667	-0.020920	0.2113
H4[1]	(0.1452, 0.3630, 0.5362)	-0.006926	-0.010622	-0.030424	0.3272
H4[2]	(0.6370, 0.7822, 0.5362)	0.010622	0.003697	-0.030424	0.3272
H4[3]	(0.2178, 0.8548, 0.5362)	-0.003697	0.006926	-0.030424	0.3272
H4[4]	(0.8119, 0.6963, 0.8695)	-0.006925	-0.010623	-0.030425	0.3272
H4[5]	(0.3037, 0.1156, 0.8695)	0.010623	0.003697	-0.030425	0.3272
H4[6]	(0.8844, 0.1881, 0.8695)	-0.003697	0.006925	-0.030425	0.3272
H4[7]	(0.4785, 0.0297, 0.2029)	-0.006926	-0.010623	-0.030424	0.3272

H4[8]	(0.9703, 0.4489, 0.2029)	0.010623	0.003697	-0.030424	0.3272
H4[9]	(0.5511, 0.5215, 0.2029)	-0.003697	0.006926	-0.030424	0.3272
H5[1]	(0.0297, 0.5511, 0.7971)	0.010623	0.003697	-0.030424	0.3272
H5[2]	(0.4489, 0.4785, 0.7971)	-0.003697	0.006926	-0.030424	0.3272
H5[3]	(0.5215, 0.9703, 0.7971)	-0.006926	-0.010623	-0.030424	0.3272
H5[4]	(0.6963, 0.8844, 0.1305)	0.010623	0.003697	-0.030425	0.3272
H5[5]	(0.1156, 0.8119, 0.1305)	-0.003697	0.006925	-0.030425	0.3272
H5[6]	(0.1881, 0.3037, 0.1305)	-0.006925	-0.010623	-0.030425	0.3272
H5[7]	(0.3630, 0.2178, 0.4638)	0.010622	0.003697	-0.030424	0.3272
H5[8]	(0.7822, 0.1452, 0.4638)	-0.003697	0.006926	-0.030424	0.3272
H5[9]	(0.8548, 0.6370, 0.4638)	-0.006926	-0.010622	-0.030424	0.3272
H6[1]	(0.9515, 0.4892, 0.6484)	-0.002795	0.000871	-0.020920	0.2113
H6[2]	(0.5107, 0.4623, 0.6484)	-0.000871	-0.003667	-0.020920	0.2113
H6[3]	(0.5377, 0.0485, 0.6484)	0.003667	0.002795	-0.020920	0.2113
H6[4]	(0.6182, 0.8226, 0.9818)	-0.002795	0.000871	-0.020920	0.2113
H6[5]	(0.1774, 0.7956, 0.9818)	-0.000871	-0.003667	-0.020920	0.2113
H6[6]	(0.2044, 0.3818, 0.9818)	0.003667	0.002795	-0.020920	0.2113
H6[7]	(0.2849, 0.1559, 0.3151)	-0.002795	0.000871	-0.020920	0.2113
H6[8]	(0.8441, 0.1290, 0.3151)	-0.000871	-0.003667	-0.020920	0.2113
H6[9]	(0.8710, 0.7151, 0.3151)	0.003667	0.002795	-0.020920	0.2113
H7[1]	(0.9950, 0.3465, 0.6893)	0.000829	-0.001233	-0.023619	0.2340
H7[2]	(0.6535, 0.6485, 0.6893)	0.001233	0.002062	-0.023619	0.2340
H7[3]	(0.3515, 0.0050, 0.6893)	-0.002062	-0.000829	-0.023619	0.2340
H7[4]	(0.6617, 0.6798, 0.0226)	0.000829	-0.001233	-0.023619	0.2340
H7[5]	(0.3202, 0.9818, 0.0226)	0.001233	0.002062	-0.023619	0.2340
H7[6]	(0.0182, 0.3383, 0.0226)	-0.002062	-0.000829	-0.023619	0.2340
H7[7]	(0.3283, 0.0132, 0.3560)	0.000830	-0.001233	-0.023619	0.2340
H7[8]	(0.9868, 0.3152, 0.3560)	0.001233	0.002063	-0.023619	0.2340
H7[9]	(0.6848, 0.6717, 0.3560)	-0.002063	-0.000830	-0.023619	0.2340
H8[1]	(0.0936, 0.4165, 0.8192)	0.007985	0.010160	-0.033772	0.3573
H8[2]	(0.5835, 0.6772, 0.8192)	-0.010160	-0.002174	-0.033772	0.3573
H8[3]	(0.3228, 0.9063, 0.8192)	0.002174	-0.007985	-0.033772	0.3573
H8[4]	(0.7603, 0.7498, 0.1526)	0.007985	0.010159	-0.033772	0.3573
H8[5]	(0.2502, 0.0105, 0.1526)	-0.010159	-0.002174	-0.033772	0.3573
H8[6]	(0.9895, 0.2397, 0.1526)	0.002174	-0.007985	-0.033772	0.3573
H8[7]	(0.4270, 0.0832, 0.4859)	0.007985	0.010160	-0.033772	0.3573

H8[8]	(0.9168, 0.3438, 0.4859)	-0.010160	-0.002174	-0.033772	0.3573
H8[9]	(0.6562, 0.5730, 0.4859)	0.002174	-0.007985	-0.033772	0.3573
H9[1]	(0.3438, 0.4270, 0.5141)	0.002174	-0.007985	-0.033772	0.3573
H9[2]	(0.5730, 0.9168, 0.5141)	0.007985	0.010160	-0.033772	0.3573
H9[3]	(0.0832, 0.6562, 0.5141)	-0.010160	-0.002174	-0.033772	0.3573
H9[4]	(0.0105, 0.7603, 0.8474)	0.002174	-0.007985	-0.033772	0.3573
H9[5]	(0.2397, 0.2502, 0.8474)	0.007985	0.010159	-0.033772	0.3573
H9[6]	(0.7498, 0.9895, 0.8474)	-0.010159	-0.002174	-0.033772	0.3573
H9[7]	(0.6772, 0.0937, 0.1808)	0.002174	-0.007985	-0.033772	0.3573
H9[8]	(0.9063, 0.5835, 0.1808)	0.007985	0.010160	-0.033772	0.3573
H9[9]	(0.4165, 0.3228, 0.1808)	-0.010160	-0.002174	-0.033772	0.3573
H10[1]	(0.3152, 0.3283, 0.6440)	-0.002063	-0.000830	-0.023619	0.2340
H10[2]	(0.6717, 0.9868, 0.6440)	0.000830	-0.001233	-0.023619	0.2340
H10[3]	(0.0132, 0.6848, 0.6440)	0.001233	0.002063	-0.023619	0.2340
H10[4]	(0.9818, 0.6617, 0.9774)	-0.002062	-0.000829	-0.023619	0.2340
H10[5]	(0.3383, 0.3202, 0.9774)	0.000829	-0.001233	-0.023619	0.2340
H10[6]	(0.6798, 0.0182, 0.9774)	0.001233	0.002062	-0.023619	0.2340
H10[7]	(0.6485, 0.9950, 0.3107)	-0.002062	-0.000829	-0.023619	0.2340
H10[8]	(0.0050, 0.6535, 0.3107)	0.000829	-0.001233	-0.023619	0.2340
H10[9]	(0.3465, 0.3515, 0.3107)	0.001233	0.002062	-0.023619	0.2340
C11[1]	(0.1535, 0.3674, 0.6470)	-0.000329	-0.001025	-0.031198	0.3076
C11[2]	(0.6326, 0.7862, 0.6470)	0.001025	0.000695	-0.031198	0.3076
C11[3]	(0.2138, 0.8465, 0.6470)	-0.000695	0.000329	-0.031198	0.3076
C11[4]	(0.8202, 0.7007, 0.9804)	-0.000329	-0.001024	-0.031198	0.3076
C11[5]	(0.2993, 0.1195, 0.9804)	0.001024	0.000695	-0.031198	0.3076
C11[6]	(0.8805, 0.1798, 0.9804)	-0.000695	0.000329	-0.031198	0.3076
C11[7]	(0.4869, 0.0341, 0.3137)	-0.000329	-0.001024	-0.031198	0.3076
C11[8]	(0.9659, 0.4528, 0.3137)	0.001024	0.000695	-0.031198	0.3076
C11[9]	(0.5472, 0.5131, 0.3137)	-0.000695	0.000329	-0.031198	0.3076
C12[1]	(0.0341, 0.5472, 0.6863)	0.001024	0.000695	-0.031198	0.3076
C12[2]	(0.4528, 0.4869, 0.6863)	-0.000695	0.000329	-0.031198	0.3076
C12[3]	(0.5131, 0.9659, 0.6863)	-0.000329	-0.001024	-0.031198	0.3076
C12[4]	(0.7007, 0.8805, 0.0196)	0.001024	0.000695	-0.031198	0.3076
C12[5]	(0.1195, 0.8202, 0.0196)	-0.000695	0.000329	-0.031198	0.3076
C12[6]	(0.1798, 0.2993, 0.0196)	-0.000329	-0.001024	-0.031198	0.3076
C12[7]	(0.3674, 0.2138, 0.3530)	0.001025	0.000695	-0.031198	0.3076

C12[8]	(0.7862, 0.1535, 0.3530)	-0.000695	0.000329	-0.031198	0.3076
C12[9]	(0.8465, 0.6326, 0.3530)	-0.000329	-0.001025	-0.031198	0.3076
C13[1]	(0.0817, 0.4068, 0.7089)	0.001486	0.001742	-0.032428	0.3203
C13[2]	(0.5932, 0.6749, 0.7089)	-0.001741	-0.000255	-0.032428	0.3203
C13[3]	(0.3251, 0.9183, 0.7089)	0.000255	-0.001486	-0.032428	0.3203
C13[4]	(0.7483, 0.7401, 0.0422)	0.001486	0.001741	-0.032428	0.3203
C13[5]	(0.2599, 0.0082, 0.0422)	-0.001741	-0.000255	-0.032428	0.3203
C13[6]	(0.9918, 0.2517, 0.0422)	0.000255	-0.001486	-0.032428	0.3203
C13[7]	(0.4150, 0.0734, 0.3755)	0.001486	0.001741	-0.032429	0.3203
C13[8]	(0.9266, 0.3416, 0.3755)	-0.001741	-0.000255	-0.032429	0.3203
C13[9]	(0.6584, 0.5850, 0.3755)	0.000255	-0.001486	-0.032429	0.3203
C14[1]	(0.3416, 0.4150, 0.6245)	0.000255	-0.001486	-0.032429	0.3203
C14[2]	(0.5850, 0.9266, 0.6245)	0.001486	0.001741	-0.032429	0.3203
C14[3]	(0.0734, 0.6584, 0.6245)	-0.001741	-0.000255	-0.032429	0.3203
C14[4]	(0.0082, 0.7483, 0.9578)	0.000255	-0.001486	-0.032428	0.3203
C14[5]	(0.2517, 0.2599, 0.9578)	0.001486	0.001741	-0.032428	0.3203
C14[6]	(0.7401, 0.9918, 0.9578)	-0.001741	-0.000255	-0.032428	0.3203
C14[7]	(0.6749, 0.0817, 0.2911)	0.000255	-0.001486	-0.032428	0.3203
C14[8]	(0.9183, 0.5932, 0.2911)	0.001486	0.001742	-0.032428	0.3203
C14[9]	(0.4068, 0.3251, 0.2911)	-0.001741	-0.000255	-0.032428	0.3203
Br15[1]	(0.4243, 0.7123, 0.3502)	0.090979	0.045615	-0.074687	1.3300
Br15[2]	(0.1967, 0.6664, 0.1667)	0.045364	0.090979	0.108808	1.5416
Br15[3]	(0.3336, 0.5303, 0.1667)	-0.090979	-0.045615	0.108808	1.5416
Br15[4]	(0.0910, 0.0456, 0.6835)	0.090979	0.045615	-0.074687	1.3300
Br15[5]	(0.8634, 0.9998, 0.5000)	0.045365	0.090979	0.108808	1.5416
Br15[6]	(0.0003, 0.8637, 0.5000)	-0.090979	-0.045615	0.108808	1.5416
Br15[7]	(0.7576, 0.3789, 0.0168)	0.090979	0.045615	-0.074687	1.3300
Br15[8]	(0.5301, 0.3331, 0.8333)	0.045365	0.090979	0.108808	1.5416
Br15[9]	(0.6669, 0.1970, 0.8333)	-0.090979	-0.045615	0.108808	1.5416
Br16[1]	(0.3787, 0.7576, 0.9832)	-0.045364	-0.090979	-0.074687	1.3300
Br16[2]	(0.0454, 0.0910, 0.3165)	-0.045365	-0.090979	-0.074687	1.3300
Br16[3]	(0.7120, 0.4243, 0.6498)	-0.045364	-0.090979	-0.074687	1.3300
O17[1]	(0.1094, 0.5107, 0.6499)	-0.004320	-0.003182	-0.042966	0.4268
O17[2]	(0.4893, 0.5987, 0.6499)	0.003182	-0.001138	-0.042966	0.4268
O17[3]	(0.4013, 0.8906, 0.6499)	0.001138	0.004320	-0.042966	0.4268
O17[4]	(0.7760, 0.8440, 0.9833)	-0.004320	-0.003182	-0.042966	0.4268

O17[5]	(0.1560, 0.9320, 0.9833)	0.003182	-0.001138	-0.042966	0.4268
O17[6]	(0.0680, 0.2240, 0.9833)	0.001138	0.004320	-0.042966	0.4268
O17[7]	(0.4427, 0.1773, 0.3166)	-0.004320	-0.003182	-0.042966	0.4268
O17[8]	(0.8227, 0.2653, 0.3166)	0.003182	-0.001138	-0.042966	0.4268
O17[9]	(0.7347, 0.5573, 0.3166)	0.001138	0.004320	-0.042966	0.4268
O18[1]	(0.2653, 0.4427, 0.6834)	0.001138	0.004320	-0.042966	0.4268
O18[2]	(0.5573, 0.8227, 0.6834)	-0.004320	-0.003182	-0.042966	0.4268
O18[3]	(0.1773, 0.7347, 0.6834)	0.003182	-0.001138	-0.042966	0.4268
O18[4]	(0.9320, 0.7760, 0.0167)	0.001138	0.004320	-0.042966	0.4268
O18[5]	(0.2240, 0.1560, 0.0167)	-0.004320	-0.003182	-0.042966	0.4268
O18[6]	(0.8440, 0.0680, 0.0167)	0.003182	-0.001138	-0.042966	0.4268
O18[7]	(0.5987, 0.1094, 0.3501)	0.001138	0.004320	-0.042966	0.4268
O18[8]	(0.8906, 0.4893, 0.3501)	-0.004320	-0.003182	-0.042966	0.4268
O18[9]	(0.5107, 0.4013, 0.3501)	0.003182	-0.001138	-0.042966	0.4268

NOTE: u_x, u_y and u_z are given in relative units. |u| is the absolute displacement given in Å

Wyckoff Position Splittings:

Atom in G	**Atom(s) in H**
Ba1	Ba1
Br15	Br16 Br15
Br16	Br15
C11	C12
C12	C11
C13	C14
C14	C13
H10	H7
H3	H6
H4	H5
H5	H4
H6	H3
H7	H10
H8	H9
H9	H8
Mn2	Mn2
O17	O18

O18	O17

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