If you have created a P1 cif file for a crystal that turns out to have a rather low space group number, the space group number nor the Hermann-Mauguin name contains sufficient information to determine the crystal unambiguously. FINDSYM will write additional information. Unfortunately, cif2cell cannot smoothly read that information. This shows up via this kind of error message:

```
***Warning: Space group operation check failed for Hall symbol Unknown (H-M symbol
P21/m2/m2/a).
Traceback (most recent call last):
  File "/home/max/.local/bin/cif2cell", line 490, in <module>
    cd.primitive()
  File "/home/max/.local/lib/python3.6/site-packages/cif2cell/uctools.py", line
293, in primitive
    self.getCrystalStructure(reducecell=True)
  File "/home/max/.local/lib/python3.6/site-packages/cif2cell/uctools.py", line
432, in getCrystalStructure
    eqsites = SymOpsHall[self.HallSymbol]
```

In order to circumvent that problem, a manual intervention is needed to modify the cif file that results from FINDSYM. Based on an example, this example tells you how.

We start from a P1 cif file for a TiPt-crystal:

```
# generated using pymatgen
data_TiPt
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.62768884
_cell_length_b   2.79714039
_cell_length_c   4.88491870
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   TiPt
_chemical_formula_sum   'Ti2 Pt2'
_cell_volume   63.23183050
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  Ti  Ti0  1  0.250000  0.500000  0.700620  1
  Ti  Ti1  1  0.750000  0.500000  0.299380  1
  Pt  Pt2  1  0.250000  0.000000  0.189705  1
  Pt  Pt3  1  0.750000  0.000000  0.810295  1
```

If we run this through FINDSYM, this is the result:

```
data_findsym-output
_audit_creation_method FINDSYM

_cell_length_a    4.6276888000
_cell_length_b    2.7971404000
```

```
_cell_length_c    4.8849187000
_cell_angle_alpha 90.0000000000
_cell_angle_beta  90.0000000000
_cell_angle_gamma 90.0000000000
_cell_volume      63.2318301747

_symmetry_space_group_name_H-M "P 21/m 2/m 2/a"
_symmetry_Int_Tables_number 51
_space_group.reference_setting '051:-P 2a 2a'
_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
1 x,y,z
2 x+1/2,-y,-z
3 -x,y,-z
4 -x+1/2,-y,z
5 -x,-y,-z
6 -x+1/2,y,z
7 x,-y,z
8 x+1/2,y,-z

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_fract_symmform
Ti1 Ti   2 f 0.25000 0.50000 0.70062 1.00000 0,0,Dz
Pt1 Pt   2 e 0.25000 0.00000 0.18970 1.00000 0,0,Dz
```

The (correct) information from FINDSYM that cif2cell will not understand, is this block:

```
_symmetry_space_group_name_H-M "P 21/m 2/m 2/a"
_symmetry_Int_Tables_number 51
_space_group.reference_setting '051:-P 2a 2a'
_space_group.transform_Pp_abc a,b,c;0,0,0
```

Replacing these lines by the following ones, will work for cif2cell :

```
_symmetry_space_group_name_Hall '-p_2a_2a'
_symmetry_Int_Tables_number 51
```

How can we obtain these lines?

- The one with `_symmetry_Int_Tables_number` can just stay as it is.
- The keyword `_symmetry_space_group_name_H-M` has to be changed to `_symmetry_space_group_name_Hall`.
- Go to http://cci.lbl.gov/sginfo/hall_symbols.html, and scroll down to the bottom where there is a long list of space groups, Hermann-Mauguin symbols and Hall symbols. Search the space group number in the first column (in our example: 51) :

```
51        P m m a       -P 2a 2a
51:ba-c   P m m b       -P 2b 2
51:cab    P b m m       -P 2 2b
```

```
51:-cba   P c m m       -P 2c 2c
51:bca    P m c m       -P 2c 2
51:a-cb   P m a m       -P 2 2a
```

Read in the cif file from FINDSYM the `_space_group.transform_Pp_abc` value: it starts with '`a,b,c`'. Search that sequence in the lines for space group 51. The regular order 'abc' will not be explicitly mentioned, so "51" is equivalent to "`51:abc`", and that's the line we need here. Read the Hall symbol in the last column: "`-P 2a 2a`". This should be the string you read in `_space_group.reference_setting`, which is indeed the case. Hence, it is this Hall symbol which you have to fill out after `_symmetry_space_group_Hall`.

With these two new lines replacing the four old ones, cif2cell will correctly read your cif file.