Balls & Sticks version 1.80beta release note

2011/05/10

Balls & Sticks (BS) version 1.77c or oldermight not generate symmetry equivalent site(s) properly for the following special cases.

CASE1: When a fractional coordinate of an atom is supposed to be a common fraction, but it is inputted as a decimal number with not enough digits.

EXAMPLE: Suppose z = 1/6 is the correct value, but z = 0.167 is used as the input to BS for the following sits:

Site	***x***	***y***	***z***
Al(1)	0	0	1/6 inputted as 0.167

When the symmetry operations (-x+y+2/3, y+1/3, z+5/6 and its inversion) are applied to this coordinate (z = 0.167), the following sites are supposed to be generated:

Site	***x***	***y***	***z***	
Al(1)	2/3	1/3	0.166333	← not displayed by earlier versions of BS
Al(1)	1/3	2/3	0.999667	← not displayed by earlier versions of BS

* If it were 0.166667, it would be sufficient digits.

CASE2: The combination of the following conditions:

- ♦ A fractional coordinate of an atom is supposed to be a common fraction, and it is inputted with sufficient decimal number.
- ♦ A coordinate of an atom, which is generated by a symmetry operation onto an input coordinate, is at x = 1 and/or y = 1 and/or z = 1.

EXAMPLE:

Site	***x***	***y***	***z***
Al(1)	0	0	1/6 inputted as 0.166667

When the symmetry operations (-x+y+2/3, y+1/3, z+5/6 and its inversion) are applied to Al(1) properly, the following sites should be generated:

Site	***x***	***y***	***z***	
Al(1)	2/3	1/3	1	
Al(1)	1/3	2/3	0	← not displayed by earlier versions of BS

REVISION (on version 1.8beta or later):

When input data of the BS have one of or combinations of these special situations, expected atoms at the unitcell edge sites (x = 0,1, y = 0,1 and/or z = 0,1) might not appear on BS properly. This problem has been solved on BS version 1.8beta or later as long as user input for "supposed to be" a common fraction coordinate is imputed with a decimal number with enough digits.

PROPER INPUTS FOR COMMON FRACTION COORDINATE:

1/6 → 0.166667

5/6 → 0.833333

1/3 → 0.333333

2/3 → 0.666667

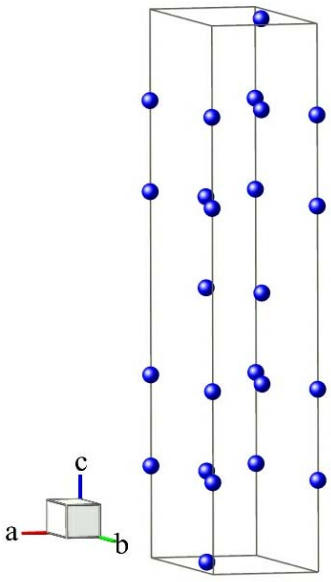
GRAPHICAL ILLUSTRATION OF THE PROBLEM AND ITS FIX

EXAMPLE:

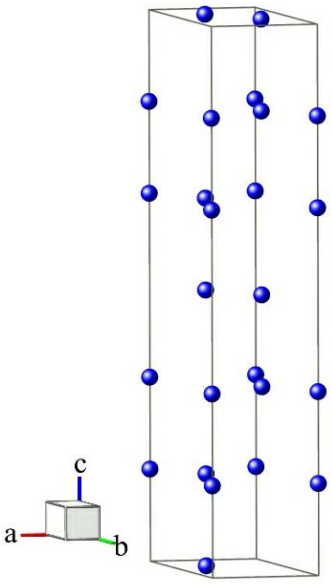
Site	***x***	***y***	***z***
Al(1)	0	0	1/6

Space group: R -3c H (167)

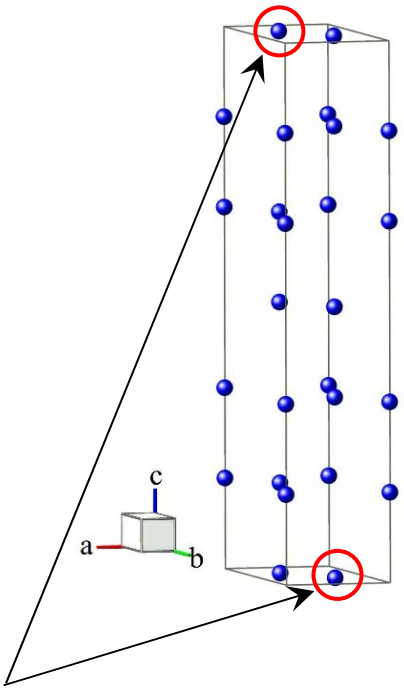
BS version: 1.77c or earlier
***z* inputted:** 0.167



BS version: 1.77c or earlier
***z* inputted:** 0.167



BS version: 1.80beta or later
***z* inputted:** 0.166667



These sites are not generated by older versions.