1) The GAUSSIAN03/09 standard links *L101* and *L502* (*l101.exe* and *l502.exe*) have to be replaced by the modified links. This can be done simply by adding the following lines before the section that starts with # in the GAUSSIAN03/09 input file (<*job_name*>*.com*):

%Subst L101 $home/ANT.G-x.x.x/bin
%Subst L502 $home/ANT.G-x.x.x/bin

where *$home* may be substituted by the appropriate directory containing **ANT.G.**

2) Set the character string in the title line of the gaussian input file <*job_name*>*.com* to whatever you like the output files to be named. You may use the same name as that of the input file (<*job_name*>). This should also be the name of the parameters file (<*job_name*>*.ini*) if you want to modify default calculation parameters (and you probably want to).

3) In order to perform standard transport calculations, part of the two metal electrodes has to be included in the atomic description of the cluster. To this end, a special convention for the coordinates specification section in the <*job_name*>*.com* input file is used so that **ANT.G** can identify the atoms to which the infinite electrodes (Bethe lattices) are attached.

Now follow these rules:

1) 3D electrodes: The first and last set of atoms in the input file should correspond to the outermost regions of the electrodes, i.e., to the ones farthest from the scattering region and should have perfect crystalline order. These should be composed of at least 2 planes each, keeping the outermost planes first and last in the input file. By default all the atoms in the outermost planes are connected to the Bethe lattice.

2) 2D electrodes: As in the 3D case, the first and last set of atoms should have perfect crystalline order. In this case, it is recommended to specify the number of atoms to be connected to the Bethe lattice in the <*job_name*>*.ini* file since, by default, it considers all the atoms in the electrodes (see below).

3) The order and atomic structure of the remaining atoms in the metallic electrodes and the molecule or rest of the system connected to the crystalline regions is not important although a standard metal-molecule-metal structure is recommended for a better analysis of the results.

With this convention **ANT.G** is able to identify the lattice directions and the atoms to which attach the Bethe lattice describing the semi-infinite electrodes. The number of atoms in the crystalline regions to be considered for connection to the Bethe lattice can be especified using the keyword *NEMBED*. You can check whether the contact to the Bethe lattice has been successful by looking at the generated *<job_name>**.**xyz* file which contains the coordinates of the original atoms and those of the ones representing the first atom of an added Bethe lattice branch. Any crystallographic directions of an fcc, hcp, or bcc structure can be used for the crystalline part of the electrodes. 2D electrodes such as graphene and 6-fold or 4-fold coordinated crystals are also accepted.

Note:
If one of the electrodes is missing you need to state this in the *<job_name>.ini* file using the electrode type GHOST (see **ANT.G** input file). The transmission is not evaluated, but the calculation is carried out similarly. If both electrodes are missing the calculation is completely equivalent to that of GAUSSIAN03/09, but using the Green's function formalism. This presents several advantages over the standard calculation.