# VB2000 Bugs

All programmes of the size and complexity of VB2000 have bugs. We need to hear from users about them so we can try to fix them.

Currently we are aware of one bug, that is very difficult to pin down. It occurs only when the directive SPHER is set to use spherical harmonics in the stand-alone or GAMESS versions. It occurs for fairly large basis sets when the memory is sufficient to run but not large enough to do the macroiterations in core. It may be related to the size of the extra group that SPHER generates. If the dimension of the SPHER group is less than 30 it seems to work fine. It is usually fairly easy to see that the macroiterations are not converging well. Increasing the memory sufficient to run in core leads to the program running normally. This is of course a problem because it is large cases where you might not have enough memory to run in core. Currently if the dimension of the SPHER group is 30 or more, the run will abort after the first macroiteration and inform you to use sufficient memory to run full in core.

One issue is with basis sets that contain h and i basis functions in a Cartesian form. This is always a bad thing to do anyway, but the GAMESS version uses Cartesian even when attempting to get a spherical harmonic result. Fortunately the Gaussian version now allows the use of pure spherical harmonics. The stand-alone version still only uses s, p and d basis functions. Work is in progress to remove this restriction. If you are using h and i basis functions, you would normally be strongly advised to (a) always use pure spherical harmonics and (b) use the Gaussian/VB2000 version. This would significantly reduce the size of the total basis and thus speed up the calculation and makes it more stable. The Gaussian version has code for Cartesian h and i basis functions, but in fact the current Gaussian itself has a bug that prevents output of the unformatted file needed by VB2000 for g, h and i functions.. The GAMESS version has the code for up to i cartesians functions, but you should normally avoid using them. The problems arise due to linear dependencies in the basis set and this seems more severe in the VB calculation than in MO calculations. The GAMESS version, when calculating CUBE files and similar, adds zero for the contribution of h and i functions, but this is a pretty good approximation.

It seems that Molden wants an molden format file that has the f coefficients in a slightly different order from GAMESS. This has been fixed in the code that outputs a Molden file. Molekel needs to be checked whether it requires the same.