

TODO List for next version of VB2000.

Below are a number of suggestions for future versions. We can not guarantee that all of them or even any of them will be in the next version. We welcome any suggestions for future improvements.

Investigate use of VB2000 as an external program for Gaussian09 version D

This may allow REACTOR runs, geometry optimisation and frequencies, along with other things.

Get extents in Gaussian version.

The integrals required in the *.dat are promised for the next Gaussian release.

Investigate effective core potential or pseudo-potential VB runs in Gaussian.

Would make it equivalent to GAMESS version.

Generate AIMPAC *.wfx files. - this is a very minor one as we already have *.wfn files

AIMAll is a good program to read wfn files

Multiwfn -- A Multifunctional Wavefunction Analyzer, seems a good program to use.

See <http://multiwfn.codeplex.com/>

TopMol can also handle *.wfn files, but also handles molden format which we already have.

Significant recoding to use features of Fortran 90.

Modules could be used in place of COMMON statements and their declarations. Would need IMPLICIT NONE for all such subroutines.

PROBABLY NOT WORTH DOING BUT "IMPLICIT NONE" IS BEING ADDED WHENEVER SIGNIFICANT CHANGES ARE MADE TO A SUBROUTINE.

Explore ways of getting a better integral package for stand-alone version.

We should look at open-source packages.

Parallelise the code.

This will not be easy, even for the GAMESS version, where we could fit in with way GAMESS does it.

Direct integrals.

Again not easy, and it may not be needed.