**Description of the files associated to ASA density gradient**

The following files are available to downloading:

Basic ASA files for different GTO basis sets

**3-21g.txt H-Kr**

**6-311.txt H-Kr**

**Huzin.txt H-Xe**

Such files are used by both f95 programs as a source of atomic ASA shape functions.

Fortran 95 source programs

**ASA\_Atomic\_Grad\_Similarity.f95**

Performs atomic calculations of density overlap and density gradient selfsimilarities.

**ASA\_Grad\_Similarity.f95**

Performs molecular calculations of density overlap and gradient similarities between two molecules which shall be described in the additional files:

**Moleculep.txt**

**Moleculem.txt**

A sample of these files is included in order to see the structure of their format.

The program allows moving one molecule with respect to the other along the z axis.