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.