Construction or Refinement of Approximate Reduced Density Matrices
Jean-Michel Gillet, Pierre Becker, Blandine Courcot, Sébastien Ragot,
Ecole Centrale Paris, SPMS UMR CNRS 8580 1, Grande Voie des Vignes, 92295 Châtenay-Malabry, France. E-mail: gillet@spms.ecp.fr

One electron density matrices (1RDM) are useful tools since they convey information concerning charge, spin and momentum densities. Their determination from ab-initio calculations is nowadays straightforward for simple systems. However, few attempts have been made to construct a semi-empirical 1RDM from data originating from different experiments [1]. One difficulty is the lack of a generic model, generalizing the Hansen-Coppens approach for charge density refinements. Furthermore, when reaching large systems, such as those encountered in biology or pharmacology, ab-initio methods turn out to be both cumbersome and sometime “too” precise [2].

After a brief review, we will propose, for those two issues, some suggestions and tracks that are or can be fruitfully explored.


Keywords: ab-initio calculations, density matrices, refinement