

The 7th MOLCAS Workshop

Uppsala University

Uppsala, Sweden

January 16-20, 2012

Welcome to the 7th MOLCAS Workshop! In this booklet you will find all the lecture notes and lab instructions which are used in the workshop. We hope that you all will have a good time here and that you will find the time well spent. Just for clarity, although this has been expressed before, the workshop is not intended to specifically teach you any quantum chemical theory but rather to instruct and familiarize you with the application of some quantum chemical methods as they are implemented in the MOLCAS quantum chemistry software package. Note, however, that there still are some few elements of quantum chemical theory in the lectures. The latter are present either because we suspect that it is instrumental for the subsequent labs or that we introduce you to some new method which you might not have been in contact with before.

On behalf of all the teachers I welcome you again to the 7th MOLCAS workshop.

Roland Lindh