To:
Prof. Dr. Gernot Frenking
Assiciate Editor
Fachbereich Chemie
Philipps-Universität Marburg
Hans-Meerwein-Strasse
D-35032 Marburg
GERMANY

From:
Robert Brotherus
Laboratory of Physical Chemistry
P.O.BOX 55
FIN-00014 University of Helsinki
FINLAND
tel. +358-9-19140306
fax. +358-9-19140279
mail: robert@iki.fi

Bologna, 4.11.1998

JCC 3160 ”Infia – a program for rotational analysis of linear molecule spectra”

Enclosed:

- Manuscript in triplicate copies
- Diskette containing the manuscript
- Diskette containing the Figures.
- Diskette submission form, filled.
- Hardcopy of the Figures.

Dear Prof. Dr. Frenking,

I have received and studied the referee comments and your own comments on the above manuscript I have submitted for publication in JCC. I have revised the manuscript accordingly and I am sending the revised version here in triplicate copies plus a diskette with a filled diskette form.

There are two main types of revisions done. One deals with the introduction of other programs and identification of main comparative advantiges of Infia. The second deals with identification and elimination of portions of the article that ”the spectroscopist does not need to be told” as commented by the other referee.

Introduction of other programs and comparison with identification of advantiges

- The introduction has been greatly expanded with the history of computer aided rotational analysis and some present programs that are used in the field (adding more references). Unfortunately, it seems, only some of the existing programs have been published. It also appears to me that many researchers still use small proprietary programs that are probably too specific and too limited in features to be published (I make a comment about this) – they can be used as a comparison though.
- The last paragraph of the introduction has been revised to give a more balanced view of the program capabilities. The advantages of the program mentioned in introduction have been moved to discussion.
- The advantiges of the Infia program were to somge degree stated already in the previous version of the manuscript. However, they were scattered around the paper in different parts. An effort has been made in this version to gather most of the statement of the advantages to the discussion chapter (extending its length) and leave the rest of the document to a more neutral description of the features. Some additions advantiges are also treated more explicitly in the discussion.
- The abstract and discussion has been modified to state the possibility of using the program for nonlinear molecules as well.
- Matter in ”Reliability of assignment” has been greatly condensed and moved to discussion since it deals with advantages of the program.

Elimination of unnecessary portions of the article

- Table 1 and Figure 15 that describe the program implementation details have been removed as requested by the other referee. I agree that they are not of interest to most of the users of the program. The chapter "Program implementation" has been also somewhat shortened.
- Figs. 8 and 10 (and references to them) have been removed. These figure showed output scripts from reduced wavenumber fit and resonance fit respectively. Since these scripts have almost the same appearance as the free parameter fit script in Fig. 7, they are not very important for the description of the program.
- Explanation of the 2B structure and some terms in the end chapter ”3.3 Transitions” have been removed. Instead, when the 2B separation is mentioned, I cite a relevant source.

- Some other practical considerations that can be considered obvious and that are not related to Infia have been removed. These include: ” However, it is common to start the analysis… isotopic species” in ”Starting the assignment…” chapter, ” When the lower state is determined… different bands” and ”One advantage of this method is that possible… will be discussed later” in ”Combination difference prediction” chapter.
- Text has been greatly shortened in the ”Fitness functions” chapter, since the chapter deals with a detail (though important one) of the program and probably is not of direct interest to most users or scientists.
- Chapter ”Building up energy level structure” was removed altogether since it deals with information that is not directly related to the program and is supposedly known by spectroscopists.

Other revisions

- The DCCBr rotational analysis article that I cite in the last paragraph of introduction as an example of the usage of the program (reference [5]) has been accepted for publication in *J. Mol. Spectroscopy* and the reference has been changed accordingly from "Submitted for publication" to ”Accepted for publication”. The exact date of its publication is not known by me at this time.

Respectfully,

Robert Brotherus