**Posudok na pracú RNDr. Miroslava Iliaša, PhD.**

**"Zahrnutie relativistických efektov vo výpoctoch vlastností chemických systémov – metódy a aplikácie"**

During the last decade the major part of the work of **RNDr. Miroslava Iliaša, PhD.** has been devoted to the development of new advanced methods for relativistic calculations of molecular structure and properties. Since there is often a substantial interplay between correlation and relativistic effects it has been obvious that the correlation effects have also to be included into developed computational approaches. Thus the author applied a variety of relativistic post-Hartree-Fock methods in his work. Still the central goal was the development of new two- and four-component relativistic approaches. In this field Miroslav Iliaš together with his co-workers has published several very original papers that are well cited and respected.

I would like to specially emphasize a few moments which are important to judge about the work in a proper perspective: a) a tremendous amount work needed for the development and implementation of new approaches, b) deep understanding of relativistic quantum chemistry and post-Hartree-Fock methods that required for this work. Thus I am glad to express my positive opinion about the research work of the applicant.

Yet, the current work is not free from formal shortcomings. For example, on page 1 the years of a few publications are missing, in References the titles of the papers are given only in small letters (even for elements of the periodical table and names of the methods), there are a few misprints; on page 15 a reference is missing, and so on. However, the mentioned above shortcomings do not affect the overall positive impression from the work.

Without doubting the scientific level of the dissertation I would be glad to learn the opinion of the author on two points listed below:

1. Do you think that two-component approaches have a serious advantage over four-component approaches with respect to efficiency? Where are the bottlenecks for two- and four-component approaches?

2. In the exact two-component approaches the remaining (large) component necessarily possesses "memory" (tails) of the small component. Does it mean that the RKB basis should be used in two-component calculations?

Záverom konštatujem, že hore uvedene skutočnosti ma vedu k jednoznačnému presvedčeniu odporučiť **RNDr. Miroslava Iliaša,, PhD.** menovanie za docenta v študijnom odbore „teoretická a počítačová chémia".

Bratislava, 15.1.2013

Vladimír Malkin, DrSc.