INFORMATION

FactSage-Teach
A thermochemical teaching program

FactSage-Teach is a thermochemical teaching program based on the FactSage application software. It comprises a disk and a comprehensive workbook. The program illustrates the practical use of thermochemistry for solving everyday problems in industry, research and environmental sciences. Through gaining a knowledge of the practical use of thermochemistry, a student is more inclined to learn the theory behind a rather dry subject matter. The workbook contains a background of the theory relating to the practical application of thermochemistry; thereafter, the assignments are given with questions and answers. The workbook also provides a quick reference guide to the software. The program is interactive and permits a user to check out 'what happens if?' by changing input parameters, and detecting the effects in the result tables or diagram output.

Introduction

FactSage-Teach, a combination of the standard version of FactSage, this handbook and a library of assignment specific small databases, is the result of a series of seminars on Computational Thermochemistry held during recent years. Many suggestions of the seminar participants have already been incorporated in both the text and the assignments. It helps everybody who uses it to understand that Computational Thermochemistry is a tool for application in day-to-day work but also a method for gaining insight into a sometimes relatively sobering theoretical subject.

The package shall help the user to practice the three step process which is always involved in the application of computational thermochemistry:

1. Analysis of the practical problem in terms of input for a calculation,
2. selection of the appropriate program module and execution of the calculation,
3. interpretation of the results in relation to the initial practical problem.

In order to execute this three step process properly the handbook provides on the one hand an outline of the theoretical background of computational thermochemistry (section I) and on the other information on the actual use of the calculation modules of FactSage (section III, together with the slide show files of FactSage). The practical assignments (section II) are embedded between these two sections. Appropriate cross-references to sections I and III are given with each assignment in section II.