The calculation of thermodynamic properties of molecules

Thermodynamic data are key in the understanding and design of chemical processes. Next to the experimental evaluation of such data, computational methods are valuable and sometimes indispensable tools in obtaining heats of formation and Gibbs free energies. The major toolboxes to obtain such quantities by computation are quantum mechanical methods and group contribution methods. Although a lot of progress was made over the last decade, for the majority of chemical species we are still quite a bit away from what is often referred to as chemical accuracy, i.e. 1 kcal mol⁻¹. Currently, for larger molecules the combination of group contribution methods with group additive values that are determined with the best available computational ab initio methods seems to be a viable alternative to obtain thermodynamic properties near chemical accuracy. New developments and full use of existing tools may lead to further improvements.

General information
State: Published
Organisations: Computer Aided Process Engineering Center, Department of Chemical and Biochemical Engineering
Contributors: van Speybroeck, V., Gani, R., Meier, R. J.
Pages: 1764 - 1779
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Chemical Society Reviews
Volume: 39
Issue number: 5
ISSN (Print): 0306-0012
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 39.42 SJR 17.633 SNIP 7.967
Web of Science (2017): Impact factor 40.182
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 35.7 SJR 15.026 SNIP 7.621
Web of Science (2016): Impact factor 38.618
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 35.79 SJR 14.214 SNIP 7.724
Web of Science (2015): Impact factor 34.09
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 32.41 SJR 13.552 SNIP 7.504
Web of Science (2014): Impact factor 33.383
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 29.14 SJR 12.697 SNIP 6.529
Web of Science (2013): Impact factor 30.425
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 29.02 SJR 15.022 SNIP 6.672
Web of Science (2012): Impact factor 24.892
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 27.54 SJR 13.297 SNIP 6.566
Web of Science (2011): Impact factor 28.76
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2