Pure Appl. Chem., Vol. 72, No. 8, pp. 1449–1452, 2000.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

PHYSICAL CHEMISTRY DIVISION
COMMISSION ON MOLECULAR STRUCTURE AND SPECTROSCOPY*
SUBCOMMITTEE ON THEORETICAL CHEMISTRY**

GUIDELINES FOR PRESENTATION OF METHODOLOGICAL CHOICES IN THE PUBLICATION OF COMPUTATIONAL RESULTS

B. SEMIEMPIRICAL ELECTRONIC STRUCTURE CALCULATIONS†

(Technical Report)

Prepared for publication by
JAMES J. P. STEWART

Stewart Computational Chemistry, 15210 Paddington Circle, Colorado Springs, Colorado 80921 USA

*Membership of the Commission during the preparation of this report (1997–99) was as follows:

Chairman: J. E. Bertie (Canada); ***Secretary:*** P. Klaeboe (Norway); ***Titular Members:*** J. E. Boggs (USA); A. M. Heyns (RSA); N. Hirota (Japan); R. S. DcDowell (USA); ***Associate Members:*** S. M. Cabral de Menezes (Brazil); J. Kowalewski (Sweden); A. Oskam (Netherlands); P. V. R Schleyer (USA); S. Tsuchiya (Japan); Q. S. Zhu (PRC); ***National Representatives:*** R. K. Harris (UK); J. P. Hawranek (Poland); R. Janoschek (Austria); P. T. Manoharan (India): J. J. C. Teixeira-Dias (Portugal); Y. S. Lee (Republic of Korea); B. van der Veken (Belgium).

Membership of the Subcommittee on Theoretical Chemistry during the preparation of this report was as follows: ***Chairman:* J. E. Boggs (USA); ***Members***: George Famini (USA), R. Janoschek (Austria), Z. B. Maksic (Croatia), I. M. Mills (UK), P. v. R. Schleyer (Germany), J. J. P. Stewart (USA), T. B. Stouch (USA).

†Part A of the Guidelines, "*Ab Initio* Electronic Structure Calculations", was published in *Pure Appl. Chem.* **70**, 1015–1018 (1998).

Guidelines for presentation of methodological choices in the publication of computational results B. Semiempirical electronic structure calculations

Abstract: Guidelines are presented to assist authors in preparing manuscripts that describe the results of semiempirical computations. These guidelines are not intended to recommend how semiempirical calculations should be done, but rather to ensure that the reader can have a clear understanding of what actually was done. They are written in a form to facilitate reprinting in original research journals and as information sheets that can be distributed to authors and reviewers.

BASIC PRINCIPLES

The basic principles are the same as for all scientific publications:

1. Give enough information to enable the reader to repeat the calculation. This is the overall guiding principle of these recommendations.
2. Give credit for all work taken from others.
3. Exercise care and courtesy and give complete references if you make comparisons to other computational or experimental work.
4. Use acronyms only when they increase the readability of a paper. All but the most common should be written out at first use.
5. Avoid reporting an excessive number of figures in computed parameters. In general, show only the number that can be anticipated to be meaningful in comparison with reality. If digits that are not significant are quoted to facilitate exact reproduction of the calculation, indicate this fact.

USE OF COMMERCIAL OR OTHER WIDELY DISTRIBUTED PROGRAMS

1. Identify the program, providing a literature reference and the version number, if any.
2. Identify the particular semiempirical method used. If the authors of the program permit changes to be made to the method, either to the set of approximations used or to the values of the parameters involved, these changes must be identified.
3. When calculations other than closed-shell restricted Hartree–Fock (RHF) are done, the type of calculation [e.g., RHF open shell or unrestricted Hartree–Fock (UHF)], should be identified. If multiconfigurational, then the size of the active space and the selected configurations used should be specified. Except for ground-state calculations, the electronic state calculated should be defined
4. In general, computed results should apply to systems at stationary points on the potential energy surface. Only in exceptional circumstances should "single-point" calculations be reported. Examples of such circumstances are:

   (i) Due to limitations on computational resources, optimization of the geometry is not practical;

   (ii) The objective of the work is to use a specific geometry (experimental, e.g., X-ray, or computational, e.g., *ab initio*), in which case the source of the geometry is important. When partial geometry optimization is performed, take care to identify the fixed and optimized parts of the geometry.

5. Identify any unusual computational difficulties, particularly in generating a self-consistent field (SCF), along with the technique that was used to solve the problem. Do not report results of calculation that failed to yield an SCF.

USE OF AN ORIGINAL PROGRAM FOR EITHER THE BASIC CALCULATION OR FOR ANALYSIS OF THE RESULTS

1. The theory should be given in sufficient detail that the reader could, at least in principle, write a program to do the same thing. If the method has already been completely described in the open literature, a reference will suffice. If it is desired to publish results in the open, refereed scientific literature, full disclosure should be demanded by the editor and reviewers.
2. In order for a new method to be valid, computed observables should be rotationally invariant.
3. For a new method, atomic parameters should vary consistently in going across the periodic table. Identify cases where this does not occur and give a reason or description.
4. Specify the quality of a new method in terms of average errors for various properties. This should be sufficiently detailed to allow a reader to understand the range of calculations that can be done.

GEOMETRY OPTIMIZATION OR FREQUENCY CALCULATIONS

1. Report any geometry constraints that may have been used. If the starting geometry was symmetric, identify that symmetry.
2. Quote the convergence limit used for geometry optimization if it is different from the default value of the program.
3. If force constants are reported, give their units and make sure the vibrational coordinates being used are clear. This is especially important for internal coordinates. Also, identify the geometry used as a reference. If Cartesian force constants are given, be sure to give the Cartesian atomic positions on which they are based.
4. Identify vibrational coordinates as mass-weighted or Cartesian.

TRANSITION STRUCTURES IN CHEMICAL REACTIONS

1. Specify whether frequency calculations have confirmed that one and only one imaginary frequency exists.
2. Specify whether explicit calculations have identified the minima linked by the transition structure.

COMPARISON WITH EXPERIMENTAL DATA

1. Give a reference to the original source of the data. If you use a data compilation, that reference may be helpful, but be sure to check the original references to verify the accuracy of the numbers. Indicate whenever data apply to condensed-phase systems.
2. Specify the nature of the experimental data with which comparison is made. Giving an experimental bond length, for example, is not acceptable unless the type of measurement and analysis are also given. X-ray diffraction measures the distance between centroids of electron density while electron or neutron diffraction measure the distance between nuclei. Electron diffraction may yield a vibrationally averaged distance while microwave spectroscopy may produce anything from an equilibrium distance (the only experimental parameter directly comparable to a computationally optimized internuclear distance) to a purely operationally defined substitution distance.
3. If the original author gives an estimated uncertainty such as 154.2(7) nm, quote the uncertainty as part of the experimental data.

4. Try to avoid vague statements such as “good agreement”. By comparison, “agreement within estimated experimental uncertainty” has more clear meaning.

ACKNOWLEDGMENTS

These guidelines incorporate suggestions from T. Hirano, A. Holder, K. Jug, J. McKelvey, H. Rzepa, K. Seddon, and W. Thiel.