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**Donald G. Truhlar, Associate Editor**

April 2, 2003

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CHILE

MS. NO.: JA028527U-3-a-280  
AUTHORS: Eduardo E. Chamorro, Pratim K. Chattaraj, and Patricio Fuentealba  
TITLE: The Variation of the Electrophilicity Index Along the Reaction Path

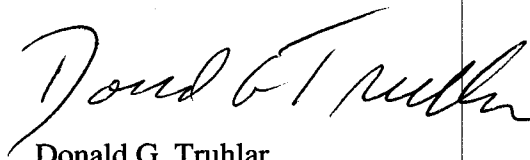
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I enclose two more referee reports. Based on these reports, I have decided not to accept this paper for publication in JACS.

Because of space limitations, JACS can accept only about 60% of the Articles and 50% of the Communications which are submitted. Since the reason for declining your paper is that it does not satisfy the general interest requirement of the Journal, you may wish to consider submitting it to another journal published by The American Chemical Society, for example the «journal». In that case, upon receiving your written request, we would be happy to forward the comments of our referees directly to that journal. It is possible that this would reduce the time required for review.

Thank you for considering JACS for publication of this work.

Sincerely yours,

  
Donald G. Truhlar  
Professor

DGT:hh  
Encl.

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2 WEEKS, PLEASE NOTIFY US IMMEDIATELY.

REFEREE D

MS NO: JA028527U-3-280

AUTHOR: Eduardo E. Chamorro\*, Pratim K. Chattaraj, Patricio Fuentealba

TITLE: The Variation of the Electrophilicity Index Along the Reaction Path

PLEASE RETURN ONE SIGNED ORIGINAL AND ONE ANONYMOUS COPY BY: MAR 13 2003

Would the article be suitable for publication: without change? YES, after minor revision? NO, after major revision? NO

Is JACS the best medium for publishing this article? NO If not, what other journal would you suggest?

J. PHYS. CHEM. A Please be as specific as possible if revision by the author is recommended. Indicate specifically whether descriptions of methods, tables of data, etc. should be reduced or eliminated with the understanding that they would be available to specialists in the form of microfilm or in some other way. Is the manuscript likely to be of interest to the broad readership of the Journal? Are the conclusions adequately supported by the data presented? Are the literature references appropriate and correct? Does the nomenclature used conform with accepted practice? Are hazardous procedures clearly defined as such?

COMMENTS:

This paper contains an interesting discussion on the behaviour of a recently introduced reactivity index, the electrophilicity, along the reaction path. The results are presented in a clear way and the paper should certainly be published. In view of the special attention devoted in JACS to the broad readership I am however more reluctant to consider this as a possible JACS publication.

I think that J. Phys. Chem. A would be the most appropriate place.

So my suggestion would be : if the two editors can arrange such an agreement, publish as such in J. Phys.Chem. A.

PLEASE SIGN THIS PAGE

Rev. 3/04

(We would also appreciate one unsigned photocopy for the author; use additional blank pages if needed.)

REFEREE E

Manuscript JA028527U-3-a-280, "The Variation of the Electrophilicity Index Along the Reaction Path"

by Eduardo E. Chamorro, Pratim K. Chattaraj, Patricio Fuentealba

Recommendation: Rejection, Publish Elsewhere

Comments:

In this version, the authors have added the plots showing the variations of the indices along the reactions paths of a few unimolecular reactions. There are still some problems with their choices:

- they considered mainly unimolecular reactions with almost symmetrical transition states. These will undoubtedly lead to a proper behaviour of the indices in the transition regions. Even so, there is no clear maximum or minimum in the saddle regions of the reported plots.
- the authors try too hard to put the "so called Principle of minimum electrophilicity". I was never convinced with the so called " Principle of maximum Hardness", and I am not with the proposed one. There are too many 'principles' put forward but are not survived, and rapidly disappeared by the severe test of time.

Suggestion for journals: Theochem, J Org Chem



## Statement of Journal policy

The *Journal of the American Chemical Society (JACS)* publishes research in all fields of chemistry. Both Articles and Communications are published, but due to restrictions on the size of the Journal not all articles that describes good scientific work can be accepted. Referees are asked to recommend for publication only papers that are of especially high scientific quality and are particularly suitable for a wide and diverse readership. Often papers that are not accepted for publication in *JACS* are well suited for publication in more specialized journals.

Communications are restricted to reports of unusual urgency, significance, and interest.

**Theoretical papers.** *JACS* seeks a wide mix of theoretical papers in all areas of chemistry. However, due to restrictions on the size of the journal and increasing submissions, the acceptance rate for theoretical papers. Authors are urged to consider the general interest criterion especially carefully before submitting papers to *JACS*.

Most methodology papers (experimental as well as theoretical) are more suited to specialized journals, but exceptions will be made for work of unusual significance. Methodology papers in *JACS* are limited to especially original advances that open significant new possibilities. Methodology papers should include one or more applications of widespread interest to experimentalists as well as theoreticians.

Theoretical applications papers that are appropriate for *JACS* include work of especially high scientific quality and originality, prototype applications to systems of broad fundamental interest, and work advancing our understanding of and making new predictions for systems of special interest from the experimental point of view.

Interest to a broad readership can be enhanced by an introduction that places the work in perspective, a concise and well organized writing style, avoidance of or explanation of jargon, and relegation of details unnecessary for the general reader to the supporting information.

The above guidelines are necessarily subjective, and editorial decisions on acceptability will place special emphasis on the criteria of high quality and interest to a broad readership.

**Supporting information.** Material especially well suited to supporting information includes tabular material that is not necessary for following the main arguments. Supporting information may include force field parameters, convergence checks, algorithmic details, Z matrices, energies in hartrees, archive files, complete tables of vibrational frequencies, and discussion of minor issues. Supporting information may optionally be submitted as an ASCII text file, which enhances its portability to various computer platforms. Four hard copies of supporting information should be submitted with the paper to facilitate refereeing (all supporting information is refereed).

**Referees.** Authors are urged to suggest persons who are qualified to referee their papers. Due to the heavy load on well-qualified referees, such suggestions are often most useful to the editor if the author suggests six or more names.

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