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October 26, 2002

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

Dear Professor Chamorro:

Your manuscript has been reviewed by two independent referees, whose comments are enclosed. Based upon these evaluations, we have decided not to accept this manuscript 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. Inevitably, some worthwhile papers must be declined. You may wish to consider submitting it to another journal published by The American Chemical Society. 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.

If you disagree with the review comments and wish to reply in detail, please revise your paper electronically and summarize the changes that have been made and/or any points on which you disagree with the referees. It is not necessary to send us a hard copy of your manuscript when you submit it electronically

Thank you for considering *JACS* for publication of this work.

Sincerely yours,

F. E. Hadley Davis for

Donald G. Truhlar
Professor
(typed & signed in his absence)

DGT:fd
Encl.

REFEREE A
Manuscript number: ja028527u-3-a-280
Manuscript title: The Variation of the Electrophilicity Index Along the Reaction Path
Corresponding author: Eduardo E. Chamorro

Recommendation: Publish after major revisions.

(1) Is the manuscript likely to be of interest to the broad readership? no
(2) Are the conclusions adequately supported by the data presented? yes
(3) Are the literature references appropriate and correct? yes
(4) Does the nomenclature used conform with accepted practice? yes
(5) Are hazardous procedures clearly defined as such? no

General Comments:
My genuine opinion is that the present work contributes mainly to the inflation of works in the area of reactivity descriptors, it is difficult to me to understand the real usefulness in practical purposes. Essentially this work is a study of a simple mathematical function. Apart the above consideration, this manuscript cannot be published at the present for the following reasons:

1) the definition of hardness in eqn(4) (the standard or the former definition) is not consistent with eqn(11), a factor of 2 is needed (depending on standard used - see below point 4)) before (mu) immediately after (=);

2) consistently with point 1) the standard (former) definition of (gamma) is 1/3 of the derivative of the standard hardness with respect to N, so a factor 3 is needed before (gamma) in eqn(11);

3) depending on the definition of f(2)(r), in eqn(12) the factor 1/2 could be 1/4;

4) one between (omega) and the derivative of (omega) with respect to N plotted in Fig. 1 must be recomputed (see point 1)); in the last few years there is a tendency to define the various indeces in terms of derivatives of the energy without factors like 1/2 for hardness and so on, of course, this creates confusion when data are taken from various sources; Fuentealba and Parr used (eta)=(1/2)(I-A) in ref. 16 from which numbers are taken, while Parr et al in ref. 6 define (omega)=(mu)^2/2(eta) as in eqn(1) of the present manuscript (!!) with (eta)=I-A [which means (omega)=(I+A)^2/8(I-A)], the authors must solve these ambiguities in all parts of the manuscript;

5) perhaps the scale for (omega) in Fig.s II-IV must be changed for the same reason;

6) eqn(5) has a wrong sign before (mu)E'N (it is a misprint eqns(6) and (7) are correct);

7) the eqn(13) is incomprehensible;

8) how can the reader reproduce the calculations on the reactions considered in the manuscript? If the IRC is already published it must be referenced otherwise in a chemistry journal details are requested;

9) the geometries at which extrema of the studied descriptors occur should be inserted in the manuscript, or, alternatively, the reaction coordinate should be explained;

10) which is the sensitivity to the method of calculation of chemical potential and hardness computed in this work for the reacting species considered?

I suggest also some other minor revisions:

1) the nuclear potential v(r) is used but it is never defined;

2) eqns(6) and (7) being similar should be put in a more symmetrical form;

3) the derivative of (omega) with respect to N looks total in `Computational details', partial in `Results and discussion' and functional in Fig. 1. Of course, it is partial so in two places a correction is needed;

4) there are some misprints in the text, references, figures, so check carefully.

The J. of the Am. Chem. Soc. has already published paper in this area of the same type so, perhaps, after a revision according to the above points it could be published.

REFEREE B
Manuscript number: ja028527u-3-a-280
Manuscript title: The Variation of the Electrophilicity Index Along the Reaction Path
Corresponding author: Eduardo E. Chamorro

Recommendation: Publish without change.

(1) Is the manuscript likely to be of interest to the broad readership? yes
(2) Are the conclusions adequately supported by the data presented? yes
(3) Are the literature references appropriate and correct? yes
(4) Does the nomenclature used conform with accepted practice? yes
(5) Are hazardous procedures clearly defined as such? Not applicable or unknown

File Attached: No
General Comments:
Review of paper ja028527u .

This paper studies the variation of the electrophilicity index recently defined by Parr et al. (JACS, 1999, 121, 1922-1924) along an arbitrary reaction path. General conditions are derived for the electrophilicity index being a maximum or minimum along a reaction path. This is illustrated with three simple reactions involving intramolecular H transfers.

The paper is suitable for publication after revision of figure III, where "eta" and "omega" have been used instead of the corresponding greek symbols.

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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.

Prior publication. Submission of a manuscript to *JACS* implies that the work has not been published elsewhere, including posting in electronic conferences or bulletin boards.

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