JACS
Journal of the American Chemical Society

Ms. No.: JA076272K
Title: Synthesis, Structure, and Conformation of Aza[1n]metacyclophanes

Dear Prof. Rajca:

On the basis of the enclosed reviews, I regret to inform you that I cannot accept your manuscript for publication in the Journal of the American Chemical Society (JACS). Enclosed please find four reviews, with a completely split decision. The detractors to the work just feel that JACS is not the appropriate journal.

In the case of your paper, my own inspection of all the reviewer's opinions leads me to a rejection due to the increasing pressure to make sure that all JACS manuscripts are of broad interest, and completely scientifically acceptable. The fact that 50% of these reviewers are concerned with these issues means that a similar percent of the general chemical community could feel the same. Perhaps after the reviewer's comments have been addressed, submission to a more specialized journal would be appropriate.

Thank you for considering JACS for this work, and I hope you understand that the large number of papers submitted precludes us from accepting any papers which have less than fully supportive reviews.

Sincerely,

Associate Editor

Enclosures: Reviews (4), Copyright Transfer Form

Reviewer 1

Manuscript Number: ja076272k
Manuscript Title: Synthesis, Structure, and Conformation of Aza[1n]metacyclophanes
Corresponding Author: Rajca

Rating
Is the Manuscript likely to be of interest to the broad readership? Yes
Are the conclusions adequately supported by the data presented? Yes
Are the literature references appropriate and correct? Yes
Does the nomenclature used conform with accepted practice? Yes
Are hazardous procedures clearly defined as such? N/A

Recommendation: Publish after minor revisions.

Additional Comments: This very nice piece of work describes the synthesis and the properties of novel azacalixarenes. These materials will be important for sensory and materials applications and the authors show for the first time how to synthesize them easily and efficiently. This manuscript should definitely be published in JACS.

There are some issues though:

1. Some typos and clerical errors. Please check ms. carefully and remove

2. Conclusion section is missing. Please put in.

3. Shorten the paper significantly. The conformational analysis could be put in the SI and only the result of the CA should be mentioned.

4. The crystal structure details should go into the SI

5. The experimental should go into the SI

6. The nmr spectra are of interest for the specialist. They should go into the SI.

After significant shortening, this very important paper should be published in JACS

Reviewer 2

Manuscript Number: ja076272k
Manuscript Title: Synthesis, Structure, and Conformation of Aza[1n]metacyclophanes
Corresponding Author: Rajca

Rating
Is the Manuscript likely to be of interest to the broad readership? No
Are the conclusions adequately supported by the data presented? Yes
Are the literature references appropriate and correct? Yes
Does the nomenclature used conform with accepted practice? Yes
Are hazardous procedures clearly defined as such? N/A

Recommendation: Publish elsewhere.

Recommendation Text: JOC

Additional Comments: This is a technically very strong paper. The reasons for conducting the studies are well laid out and the end application are likely to be very interesting. The level of characterization of the synthetic products is well beyond standard practice and the conformational studies are detailed. However, the appeal of synthesizing a new class of metacyclophanes is not broad enough to engage the general readership of JACS and a more specialized journal is appropriate.

Reviewer 3

Manuscript Number: ja076272k
Manuscript Title: Synthesis, Structure, and Conformation of Aza[1n]metacyclophanes
Corresponding Author: Rajca

Rating
Is the Manuscript likely to be of interest to the broad readership? Yes
Are the conclusions adequately supported by the data presented? Yes
Are the literature references appropriate and correct? Yes
Does the nomenclature used conform with accepted practice? Yes
Are hazardous procedures clearly defined as such? N/A

Recommendation: Publish after minor revisions.

Additional Comments: The authors describe the syntheses, structural characterization and conformational analysis of some new aza[1n]metacyclophanes. The paper is very well-written and was a pleasure to review. The work is of broad interest; appealing to individuals working in material science, physical organic chemistry and supramolecular chemistry (particularly calixarene chemistry). In addition, the experimental section and supporting documentation are impeccably detailed. While the two separate synthetic protocols and structural analyses are significant contributions, the greatest importance is the conformational studies for the macrocyclic compounds in solution. Prior to these studies that aspect of aza[1n]metacyclophanes was unexplored. The battery of analytical techniques employed (FAB MS, X-ray diffraction, molecular dynamics calculations, Gel permeation chromatography, light scattering, 1H and 13 C NMR spectroscopy) fully describes and characterizes the structures. The conclusions drawn from these studies are consistent with the data. In summation, the authors are to be congratulated on a significant scientific contribution and publication in the Journal of the American Chemical Society is completely warranted. The paper should be published without any major revisions. There are some formatting issues on line 3 of the acknowledgement section.

Reviewer 4

Manuscript Number: ja076272k
Manuscript Title: Synthesis, Structure, and Conformation of Aza[1n]metacyclophanes
Corresponding Author: Rajca

Recommendation: Publish Elsewhere.

Additional Comments: This paper represents a tour de force in synthesis and characterization. The authors have created a new class of cyclophanes that have analogies to calixarenes. These structures may prove to be interesting hosts.

However, having stated the novelty, the question is whether the work is proper for JACS and a general audience. Really, only molecular recognition and host-guest chemists will be interested in this work. Therefore, the paper should be in a specialized journal.