Dear Prof. Ivan Oskar Juranic,

We have now revised our manuscript by incorporating the Grimme's dispersion (B3LYP-D3 & B3LYP-D3(BJ)) in our calculations as suggested by the reviewer.

Hope this revised version meets the expectation of the reviewer. We express our thanks for considering this manuscript for a possible publication in your journal. We shall be looking forward to hearing from you in due course.

|  |  |  |
| --- | --- | --- |
| S.No. | Comments from the Reviewer A | Reply from the Author |
| 1. | I'm satisfied with all changes authors had been made, except with the fact that dispersion contribution have been neglected, even in revised manuscript, although both Reviewers pointed out its necessity.  However I could not recommend manuscript for publication without additional results, which may lead to different conclusions. Computing facility cannot be limiting factor, since I do not ask for huge basis set (I recommend to keep the same they used), and adding Grimme’s dispersion is not computationally demanding. | 1. The authors gratefully acknowledge this useful remark made by the reviewer and for providing valuable comments for the improvement of the paper. We appreciate the reviewer's concern and the suggested amendment has been addressed by incorporating the Grimme's dispersion (B3LYP-D3 & B3LYP-D3(BJ)) in our calculations. We have incorporated the values obtained by using B3LYP-D3 & B3LYP-D3(BJ) level in Table I in the manuscript.  2. The values obtained via all the levels are quite comparable to each other and also the trends among the cations under study remains the same. we feel that our objective of the study is to focus on the chemistry behind the problem and we are more specific about the variation in trends. Although the incorporation of dispersion functions have meagre effects on the magnitude of the parameters under study, we now believe that the data in the modified manuscript were reliable enough to discuss the chemistry behind the problem under study.  3. The recommended changes has been carried out and highlighted in page 3,5 & 13.  4. References regarding the Grimme's dispersion function has also been included in reference section as Ref. 37 and 38 and highlighted in page 13. |