Dear Reviewers,

Thank you so much for reviewing of my manuscript entitled:” A theoretical study on the *regio*- and *stereoselectivity* of [3+2] cycloddition of β- trifluoroacetyl vinyl ethyl ether with 3-oxo-1,2-pyrazolidinium ylides”. We read your comments carefully and try to revise it according to your recommendations. All changes in the text were highlighted by blue. Please find in the following some responses

**Reviewer 1:**

-The mentioned items are changed to italic font according to your comment.

-We try to revise the whole of manuscript and correct typesetting errors according to your recommendations

**Reviewer 2:**

1-In the experimental work , [Ref. 25] this reactions is indicated as 1,3-dipolar cycloaddition reaction but we replaced 1,3-dipolar cycloaddition to [3+2] cycloaddition reactions according to your recommendations.

2-“concerted’ is replaced by “one-step” according to your recommendation.

3-In the work of Xin and et al., they used unsymmetrical reagents therefore the reactions are asymmetric.

4-As you recommended FMO theory removed from the text.

5-We recalculate the reactivity indices for compound 1 as an example at the B3LYP/6-31G(d) level, which is shown in below. As can be seen from the table, there is not any significant differences between those calculated by B3LYP/cc-pVDZ and B3LYP/6-32G(d). Therefore there is not necessary to recalculate these values for others to saving the time.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | ***Species*** | | ***EHOMO*** | ***ELUMO*** | ***µ*** | ***η*** | ***ω*** | ***N*** |
| **at B3LYP/cc-pVDZ** | **1** | -0.25715 | | -0.06967 | -4.431 | 5.083 | 1.930 | 2.183 |
| **at B3LYP/6-31G(d)** | **1** | -0.25316 | | -0.06488 | -4.327 | 5.123 | 1.8267 | 2.290 |

6-Alought we agree with your comments but there are some reports that used parr functions for accounting the regioselectivity for nonpolar therefore since our studied reactions are low polar then we preferred to use parr functions analysis.

For example:

RSC advances, 2015,5, 99299-99311.

Molecular Physics 2015, 113,

7- The reference no 25 is corrected.

8-Some explanations were added about rate determining step of reaction in the text.

9-The reaction Gibbs free energies and enthalpies are given in supporting data to saving the lengths of article.

10, 13 and 14-. All mentioned mistakes are corrected in the revised version of manuscript according to your recommendation.

11-The nucleophilicity index equation is corrected.

12-Definition of IRC and GEDT are corrected in the text.

**Reviewer 3**

-The mentioned page number is corrected.