Response to Reviewer

1. We have now critically checked the experimental FT-IR for both the compounds and do admit that both of recorded a strong absorption peak around 2360 cm-1. We have also verified the chemical structures and do confirm that this particular IR absorption peak is not characteristic to any of the chemical structures and that’s why theoretical calculations did not record any such peak. We completely do agree with the views of the learned reviewer that this is an extra peak in both the experimental FT-IR spectra arisen due to aerial (atmospheric) carbon dioxide, the molecules of which remained present on the walls of the pores of potassium bromide (KBr) pallet (disc) – truly speaking these carbon dioxide molecules were encapsulated within the pores of the walls of KBr disc during sample preparation --- this an experimental error indeed. We have now mentioned this issue with the revised manuscript for the readers (Line 163-166).
2. ’optimize’ has been changed to ‘optimized’ (Line 151).
3. Random has been changed to Radom in Ref.10 (Line 392).
4. ‘A.J.A. Bienko’ has been changed to ‘A.J.Abkowicz-Bienko’ in Ref. 15 (Line 401).
5. Ref. 30 has been dully completed.