Response to Editor

1. AD1: We have moved Fig.5 to SI as Fig. S10.
2. AD2: Running title has been reduced.
3. AD3-AD10: We have converted all the figures in tif format and also removed their frames.
4. AD6-AD8: We have addressed comments accordingly regarding units and font size.
5. AD11: Reference 12 has been dully completed.
6. AD12: Reference 14 has been checked.
7. AD13: ISBN No. has been included in reference 16.
8. AD14: Fig. S1 (a) to S1 (d) and S2 (a) to S2 (d) of SI have assigned unique No S1 to S8.
9. 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 147-150).
10. ’optimize’ has been changed to ‘optimized’ (Line 135).
11. Random has been changed to Radom in Ref.10 (Line 376).
12. ‘A.J.A. Bienko’ has been changed to ‘A.J.Abkowicz-Bienko’ in Ref. 15 (Line 384).
13. Ref. 30 has been dully completed.