Our response to the reviewer’s comments:

The authors would like to appreciate the reviewer’s professional comments. Here are the replies to the questions:

1. Line 38. Here it would be useful to mention the energy cut-off and the number of K-points previously used to perform the energy calculation.

   Response:
   We inserted a sentence as below (in red) to account for the energy cut-off and K-point, please see the revised manuscript in line 43.

   *The energy cut-off was set as 750 eV and the K-point separation was 0.07/Å. Norm-conserving pseudopotentials …*

2) Line 45. The meaning of the sentence “… locations of 50% possibility were labelled.” is unclear. Please, clarify it.

   Response:
   The hydrogen atoms in crystal are disordered. Each hydrogen atom has two possible positions along the O…O chain, and each position has a 50% probability. We deleted this sentence due to its ambiguous.

3) Line 54. Here it is not clear which hydrogen-bond property is underestimated by the RPBE functional. In case it underestimates hydrogen-bond distances only, the theoretical crystal density should be higher than the experimental one, which is not the case. Please, clarify this point.
Response:
The RPBE function slightly underestimate the H-bond force. Thus the length of H-bond increases. That’s why the density is lower than experimental data.

4) Line 173. I think that the 3N-3 rule was not found firstly in this work, as it was largely used in previous studies of the same authors. Better rather emphasize it was confirmed.

Response:
Thank you very much for your elaborate review. According to solid state theory, to calculate the lattice vibrating phonons, there are 3N-3 optic branches under Harmonic approximation. We thus obtained 3N-3 normal modes. N means atom numbers in one primitive cell. In this study, N means one molecules. So the normal modes are $3N \times 3 – 3$. For the translational region, there are 3N-3 normal modes. This rule was found by the first author, Ze-Ren Wang, and maybe cited in our other papers.