Comment on egusphere-2022-93
Anonymous Referee #1

Referee comment on "Modeling approaches for atmospheric ion–dipole collisions: all-atom trajectory simulations and central field methods" by Ivo Neefjes et al., EGUsphere, https://doi.org/10.5194/egusphere-2022-93-RC2, 2022

This manuscript explores the collision dynamics of eight ion-dipole systems using potential of mean force (PMF) calculations and molecular dynamics (MD) simulations. Collision probability maps are obtained by MD to determine the dynamic collision cross sections. The collision rate coefficient results obtained by PFM and MD are compared to the classic Su and Chesnavich and the Langevin-Gioumousis-Stevenson models. The manuscript is in general well written and well organized and manages to provide an understanding of the conditions that PMF calculations and central field models can be used reliably for the determination of the collision rate coefficient.

To further improve the manuscript, I suggest adding a comment on how long the clusters are traced after collision, i.e. what is the lifetime of the clusters shown here. In addition, the value of the probability, $P(v,b)$, at which the dynamic collision cross sections of Fig. 4(e-h) and Fig. 5(e-h) were obtained by MD, should be provided.