Supporting Information

Thermal decomposition of ammonium perchlorate-based molecular perovskite from TG-DSC-FTIR-MS and ab initio molecular dynamics

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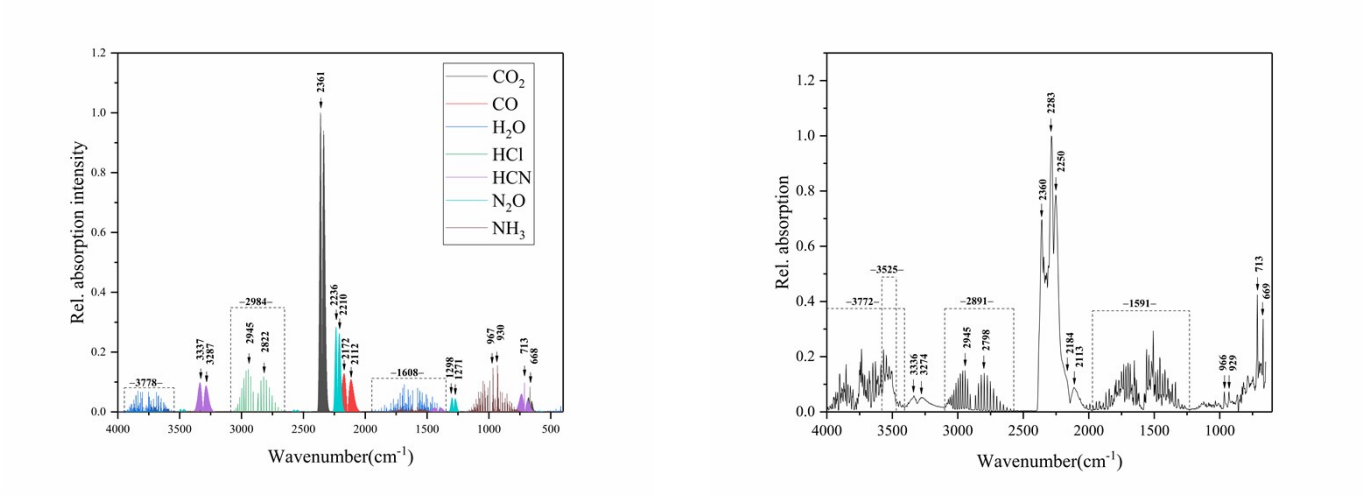
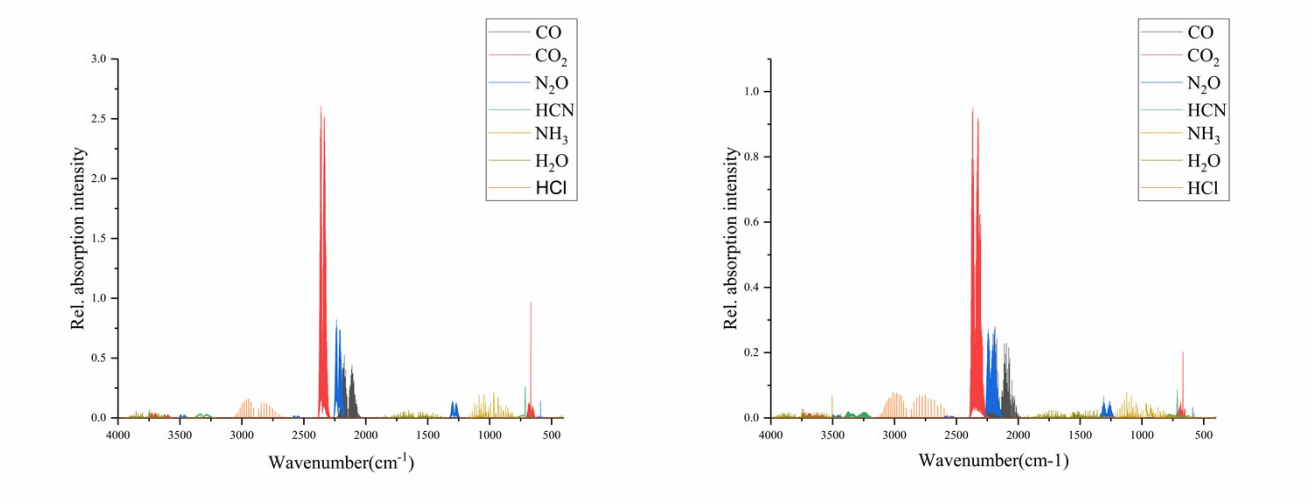


(a) (b)

Fig. S1 Identification of gas products. By comparing IR characteristic peaks of gas products for DAP decomposed at 381.8 ℃ (a) with the standard gas IR data obtained from HITRAN2016 molecular spectroscopic database[1] (b), the gas components can be clearly identified to include CO_2, CO, H_2O, HCl, HCN, NH_3.



(a) (b)

Fig. S2 Broadening of IR characteristic peaks induced by high temperature. Compared with the IR characteristic peaks at 296 K (a), IR characteristic peaks at 655 K have been broadened, but the central locations are almost unchanged.

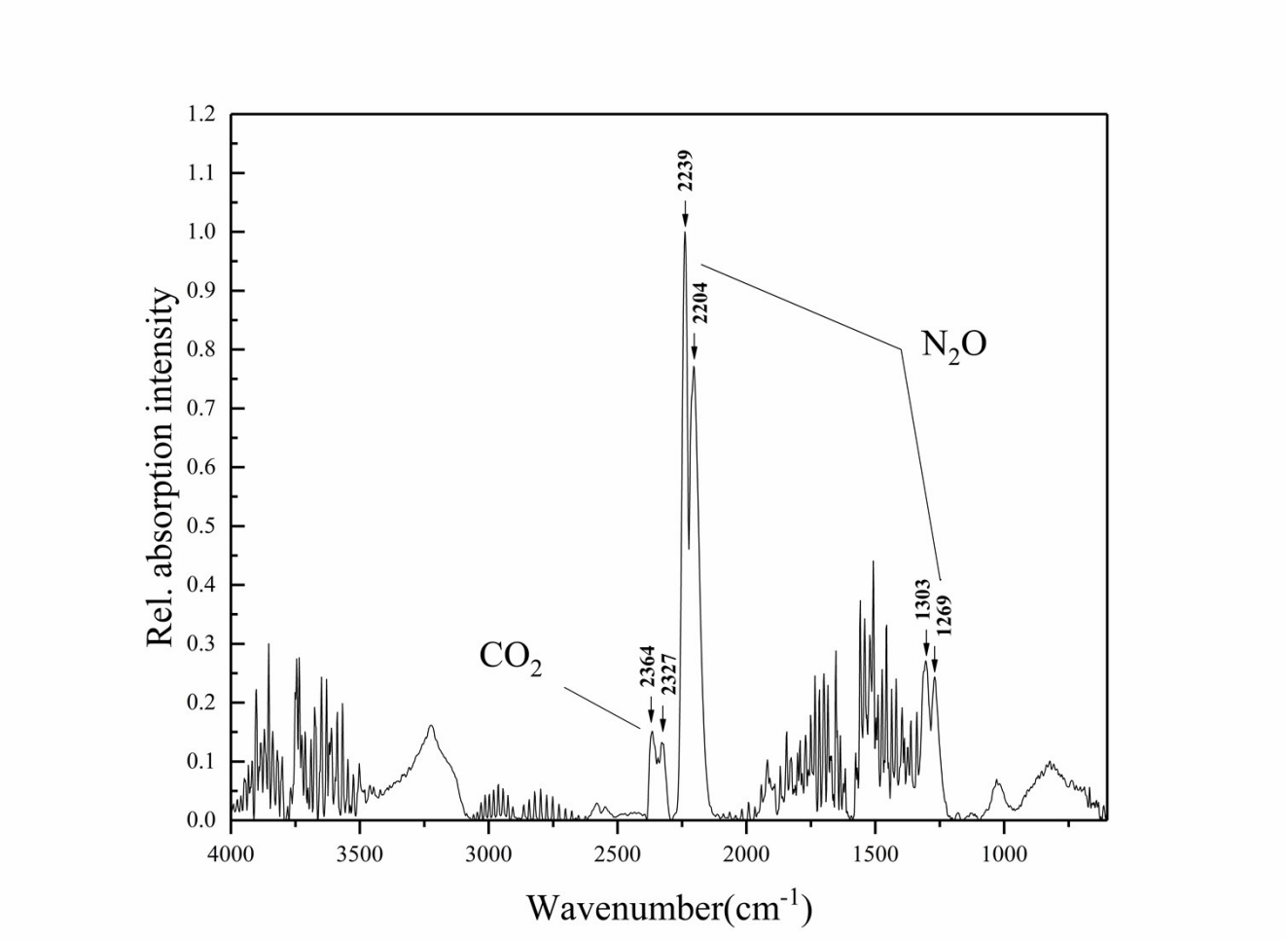


Fig. S3 IR characteristic peaks of gas products for AP decomposed at 394.8 ℃.[2] (Small amount of CO_2 comes from background gases)

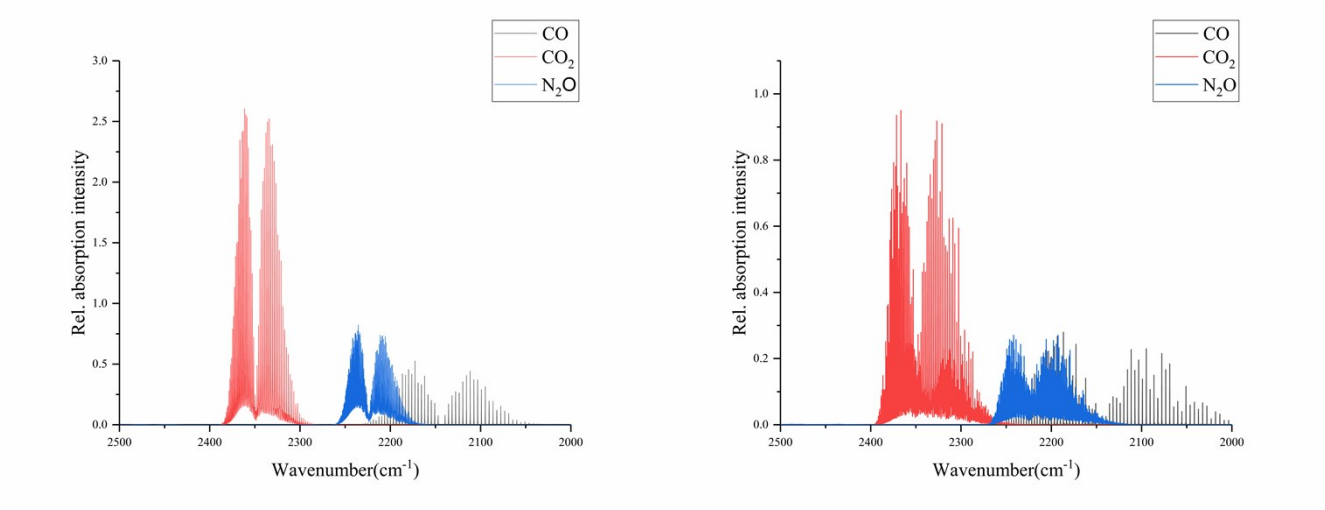


Fig. S4 Overlap of IR characteristic peaks induced by high temperature for CO_2, N_2O and CO. The IR characteristic peaks of CO_2 and N_2O are clearly not overlapped both at 296 K (a) and 655 K (b).

References:

1 P. Deng, H. Wang, X. Yang, H. Ren, Q. Jiao, J. Alloys Compd. 827 (2020) 154257.

2 I. E. Gordon, L. S. Rothman, C. Hill, et al., J. Quant. Spectrosc. Radiat. Transf., 2017, 203, 3–69.

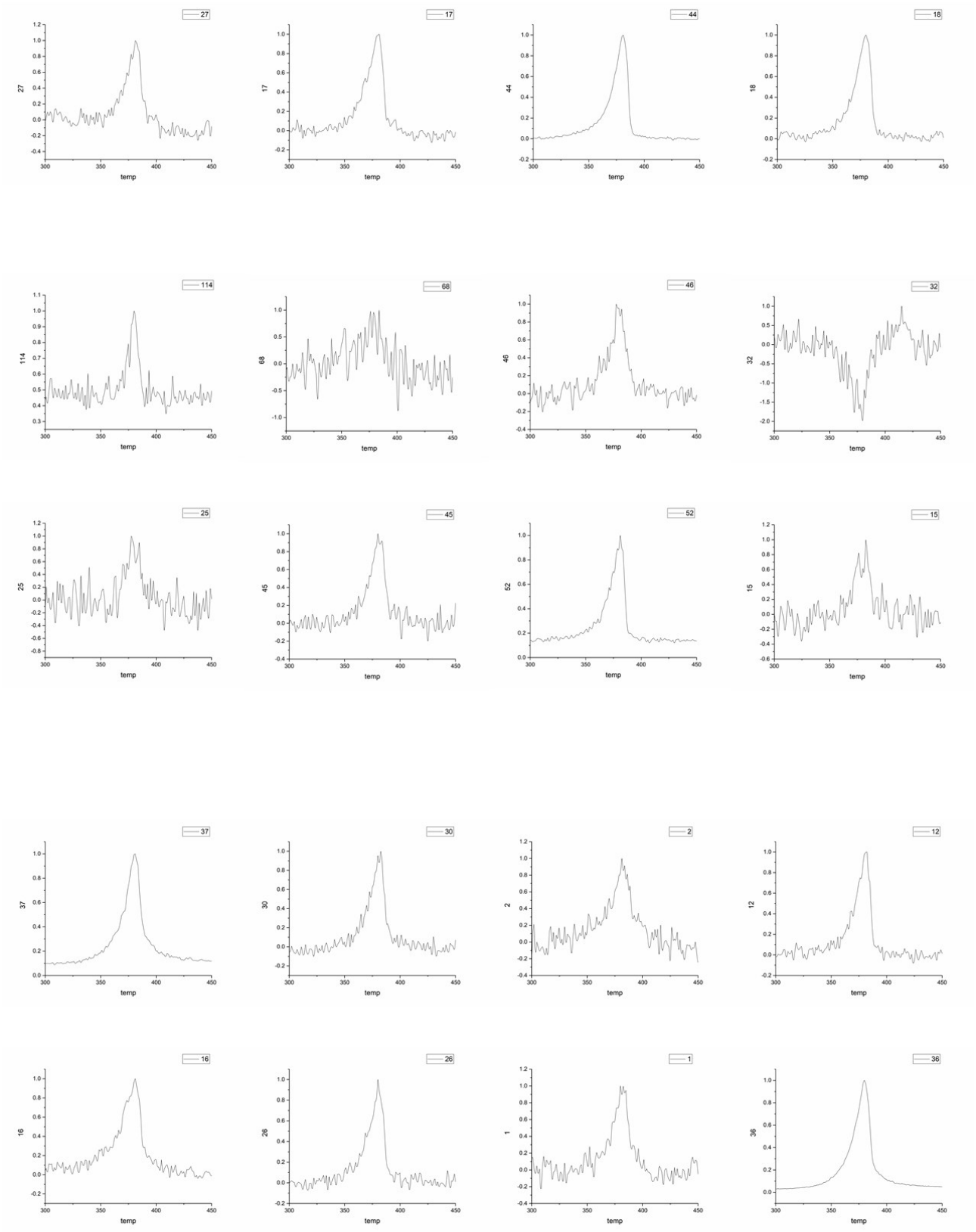


Figure S5 Evolution of product fragments from MS for DAP decomposed at the heating rate of 10 ℃/min.

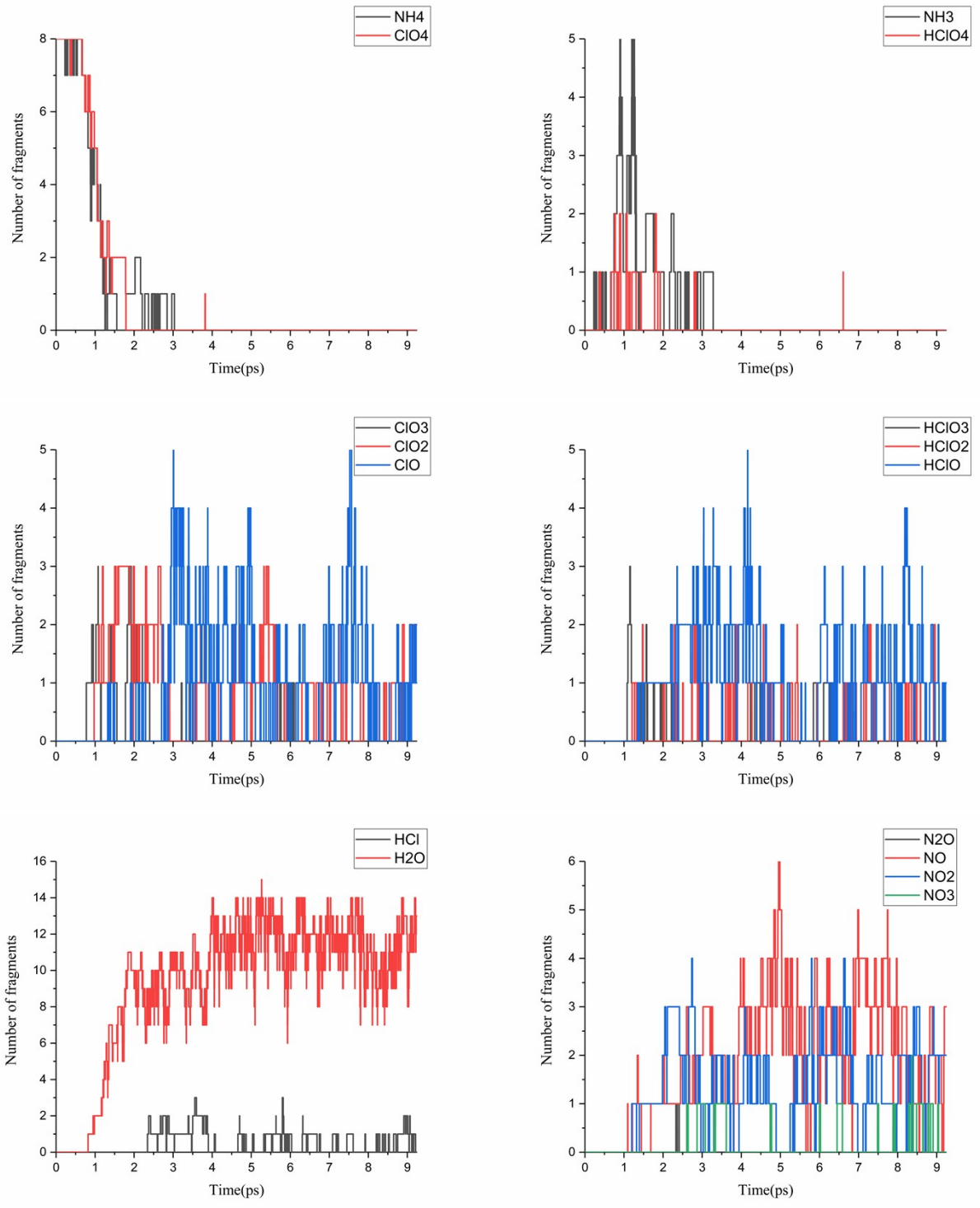


Figure S6 Evolution of key chemical species for AP decomposed at 3000 K.

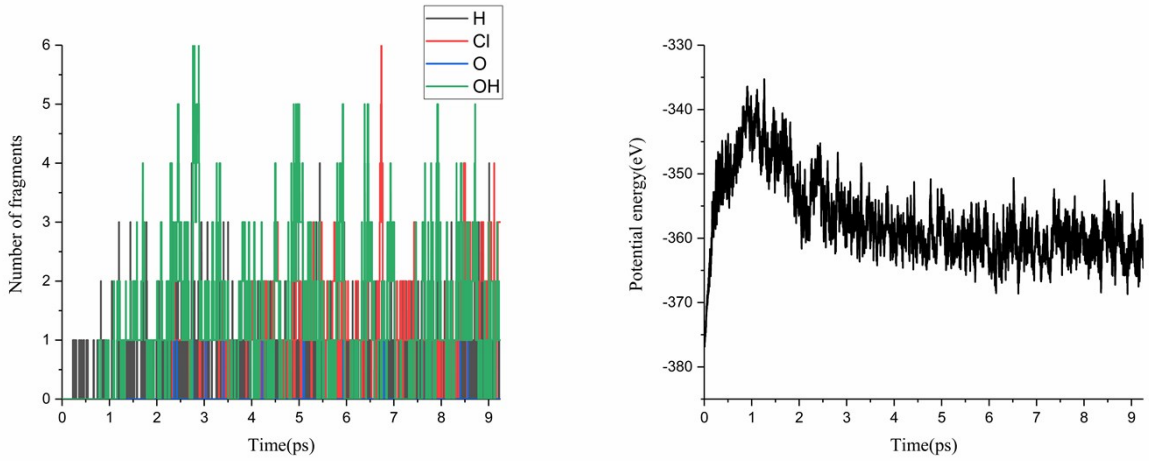


Figure S7 Evolution of free radicals and potential energy for AP decomposed at 3000 K.