

Supporting information (SI)

Uncovering the decomposition mechanism of nitrate esters plasticized polyether (NEPE): A neural network potential simulation

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In the supplementary information, we present:

- **Fig. S1** Statistics of all sampled energy and force of PEG, NG, BTTN, NG-BTTN, and PEG-NG-BTTN in NNP training within the temperature range of 300-4000 K.
- **Fig. S2** Minor gaseous species produced during the decomposition of PEG (a), NG(b), BTTN (c), NG-BTTN (d), and PEG-NG-BTTN (e) predicted by the NNP model.
- **Fig. S3** Gaseous species generated during the decomposition of NEPE matrix different mass ratios 1:2:2 (a), 1:1:1 (b), and 2:1:1 (c) of PEG, NG, and BTTN components predicted by the NNP model. Left and right subplots represent the major and minor species, respectively.
- **Fig. S4** Temporal dynamics trajectories of decomposition and the formation of intermediates and products during the thermal decomposition processes of NG (a) and BTTN (b) in the NG-BTTN plasticizer.

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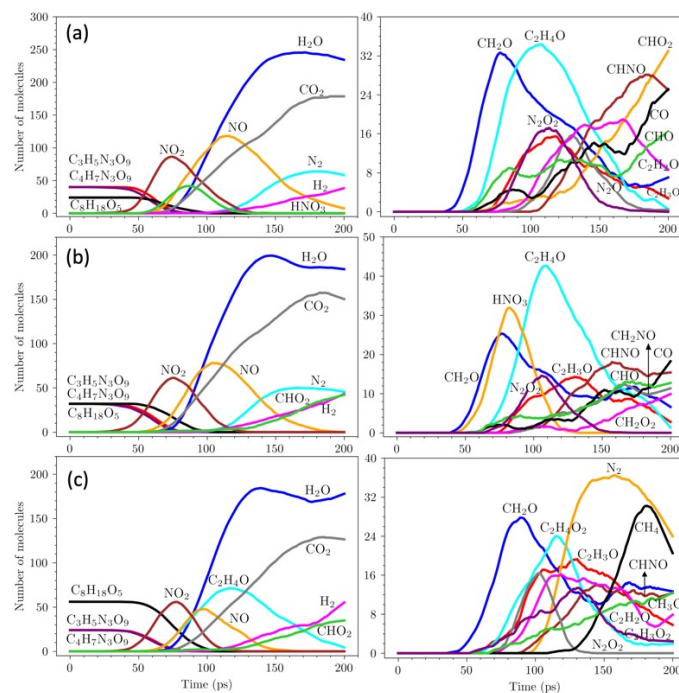


Fig. S3 Gaseous species generated during the decomposition of NEPE matrix different mass ratios 1:2:2 (a), 1:1:1 (b), and 2:1:1 (c) of PEG, NG, and BTTN components predicted by the NNP model. Left and right subplots represent the major and minor species, respectively.

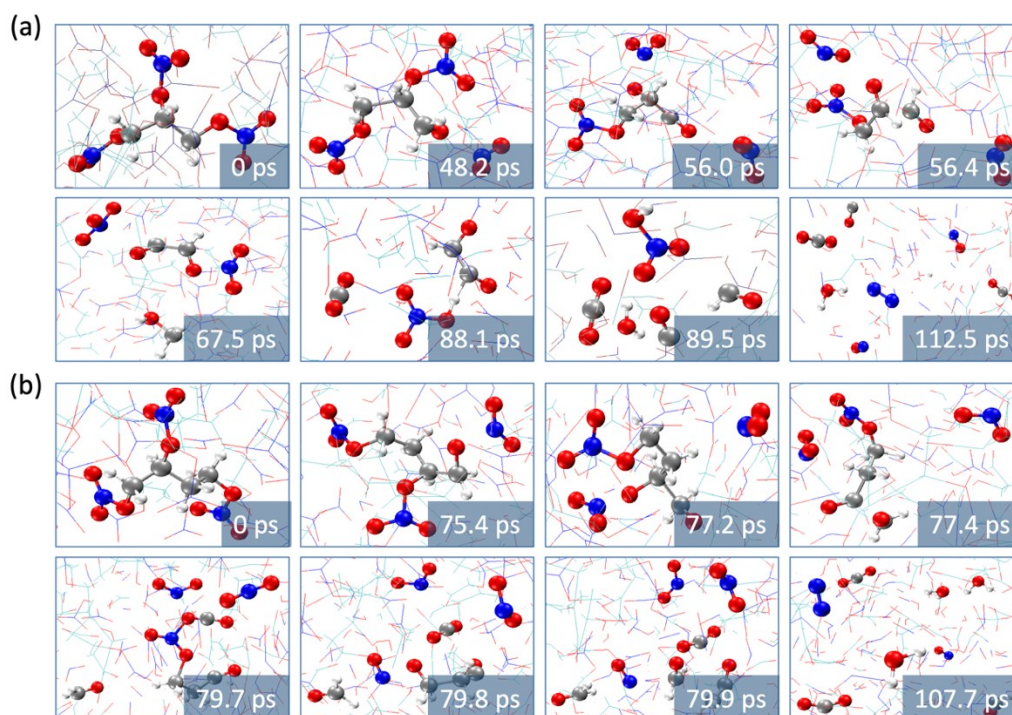


Fig. S4 Temporal dynamics trajectories of decomposition and the formation of intermediates and products during the thermal decomposition processes of NG (a) and BTTN (b) in the NG-BTTN plasticizer.