Supporting Information:

Hypergolicity of Cyanoborohydride Ionic Liquids with H_2O_2 and HNO_3 as Oxidizers in the Liquid Phase

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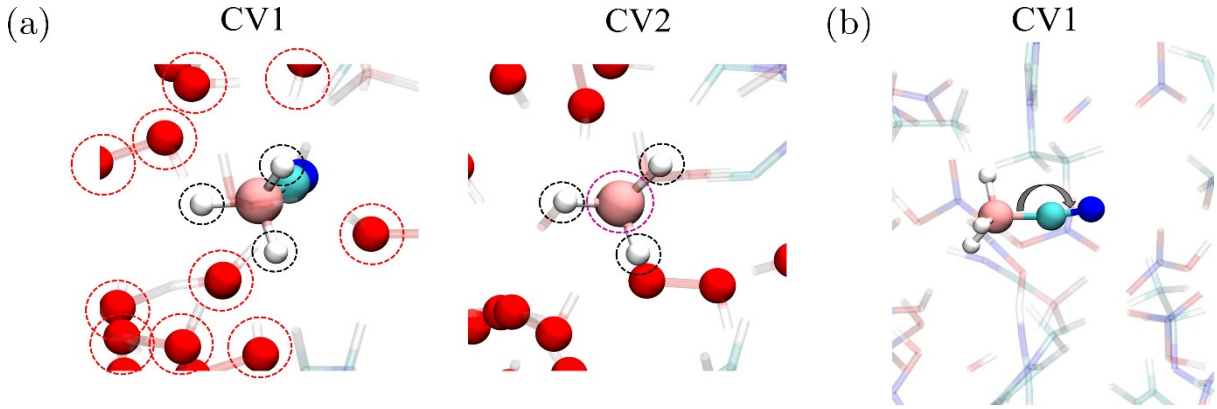


Figure S1 Collective variables used for metadynamics simulations for (a) IL + H_2O_2 – CV1: coordination number between the three H-atoms of CBH^- and the O-atoms of all H_2O_2 molecules, and CV2: coordination number between B and the three H-atoms of CBH^-, and (b) IL + HNO_3-CV1: ∠BCN.

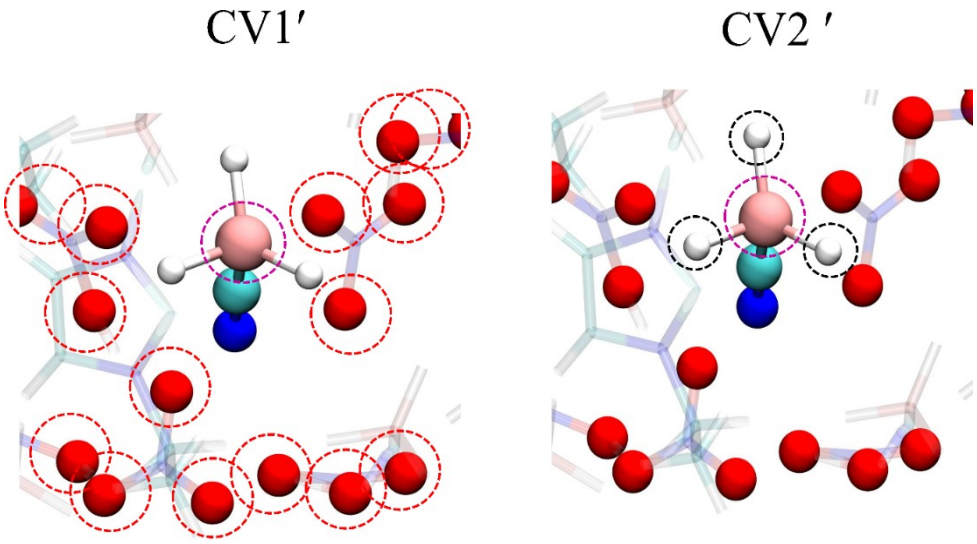
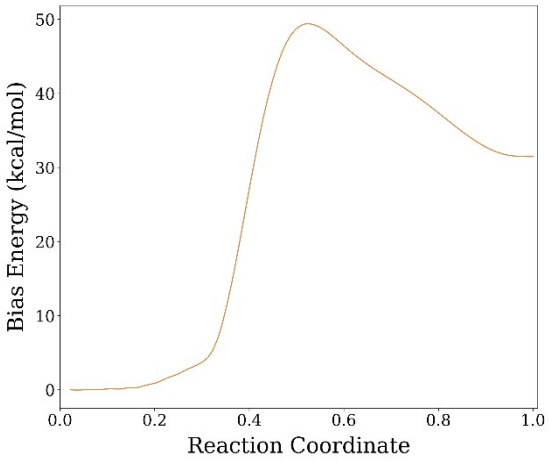


Figure S2 Collective variables used for metadynamics simulations for (a) IL + HNO_3 – CV1': coordination number between the three B-atom of CBH^- and the O-atoms of all HNO_3 molecules, and CV2': coordination number between B and the three H-atoms of CBH^-.

(a)



(b)

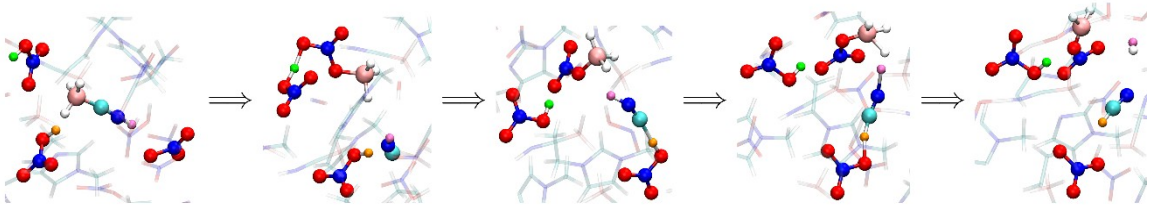


Figure S3 Bias energy for a representative trajectory as a function of CV1': coordination number between B and the three bonded H-atoms in CBH^- and CV2': coordination number between B atom of CBH^- and the O-atom present in all HNO_3 molecules in the system and (b) snapshot of the trajectory showing reaction mechanism for the formation of H_2B-ONO_2, HCN, and H_2.

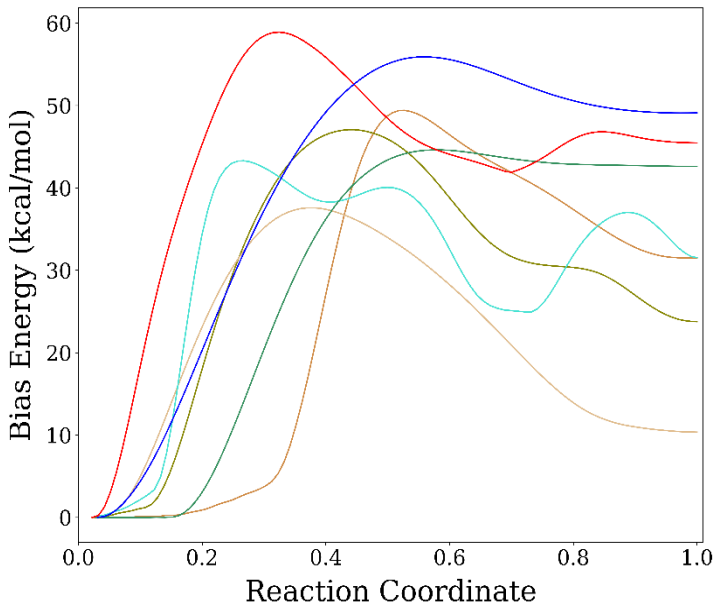


Figure S4 Bias energy as a function of CV1': coordination number between B and the three bonded H-atoms in CBH^- and CV2': coordination number between B atom of CBH^- and the O-atom present in all HNO_3 molecules in the system for a total of seven reactive trajectories initiated.