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Proton transport mechanism of imidazole, triazole and phosphoric acid mixtures from *ab initio* molecular dynamics simulations[†]

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Fig. 1 Evidence of nonconstructive ((a) for PA-TRZ system and (b) for PA-IMD system) and constructive ((c) for PA-TRZ system and (d) for PA-IMD system) proton transport. Y axis represents protonated PA's indices and the state in between two PAs are intermediate where proton is shuttling in between two PAs as shown schematically

Movie S1: Proton transfer from imidazole⁺ to imidazole in phosphoric acid-imidazole system.

Movie S2: Proton transfer from triazole to phosphoric acid in phosphoric acid-triazole system.

Movie S3: Proton transfer from triazole to phosphoric acid in phosphoric acid-imidazole-triazole system.