**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.