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Supporting Information

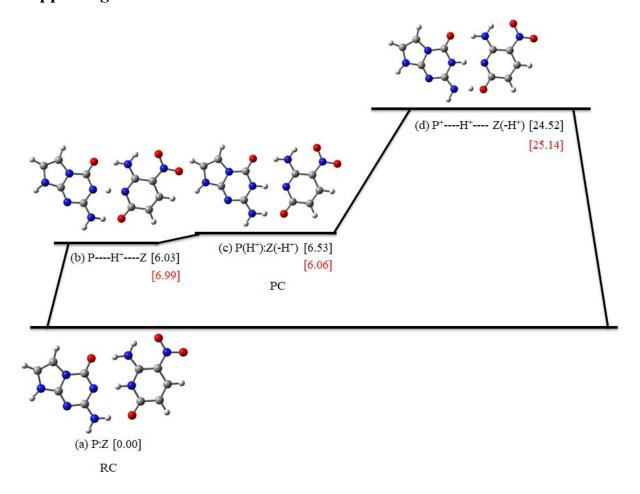


Fig. S1: Potential energy surface of the proton transfer reactions in the P:Z complex. The relative ZPE-corrected barrier energies and thermal energy-corrected Gibbs free energies (in red) are also shown.

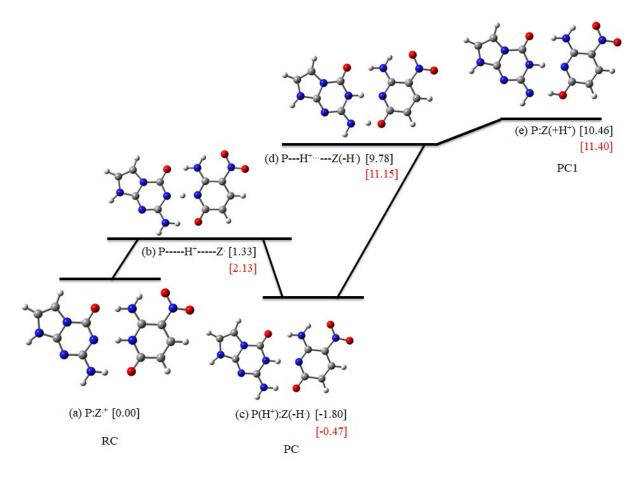


Fig. S2: Potential energy surface of the proton transfer reactions in the P:Z⁺ complex. The relative ZPE-corrected barrier energies and thermal energy-corrected Gibbs free energies (in red) are also shown.

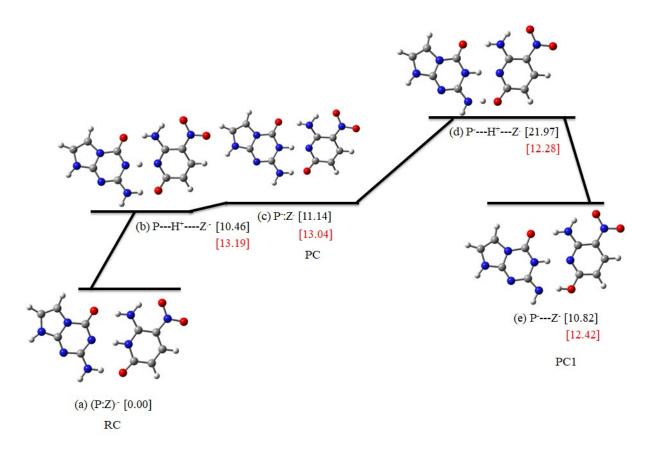


Fig. S3: Potential energy surface of the proton transfer reactions in the P:Z- complex. The relative ZPE-corrected barrier energies and thermal energy-corrected Gibbs free energies (in red) are also shown.