

Supporting Information

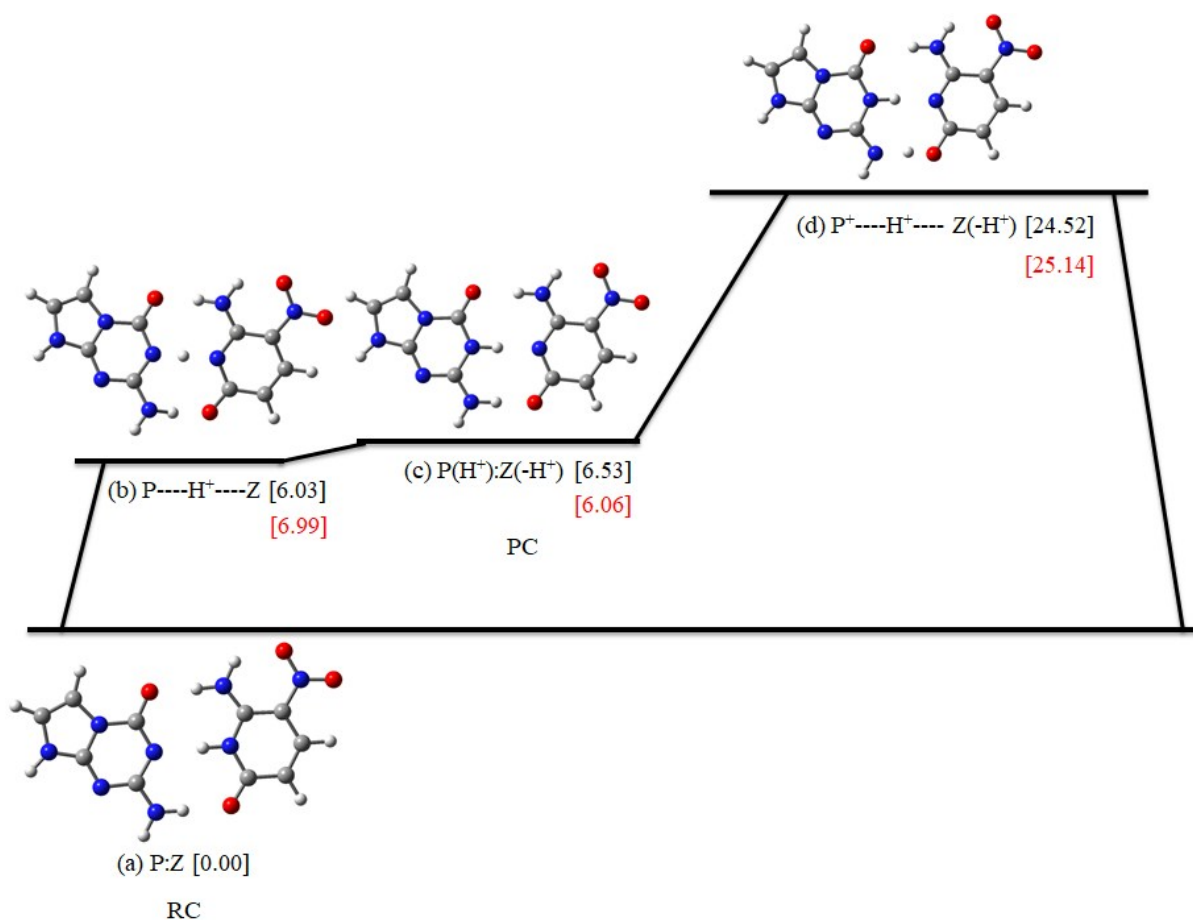


Fig. S1: Potential energy surface of the proton transfer reactions in the P:Z complex. The relative ZPE-corrected barrier energies and thermal energy-corrected Gibbs free energies (in red) are also shown.

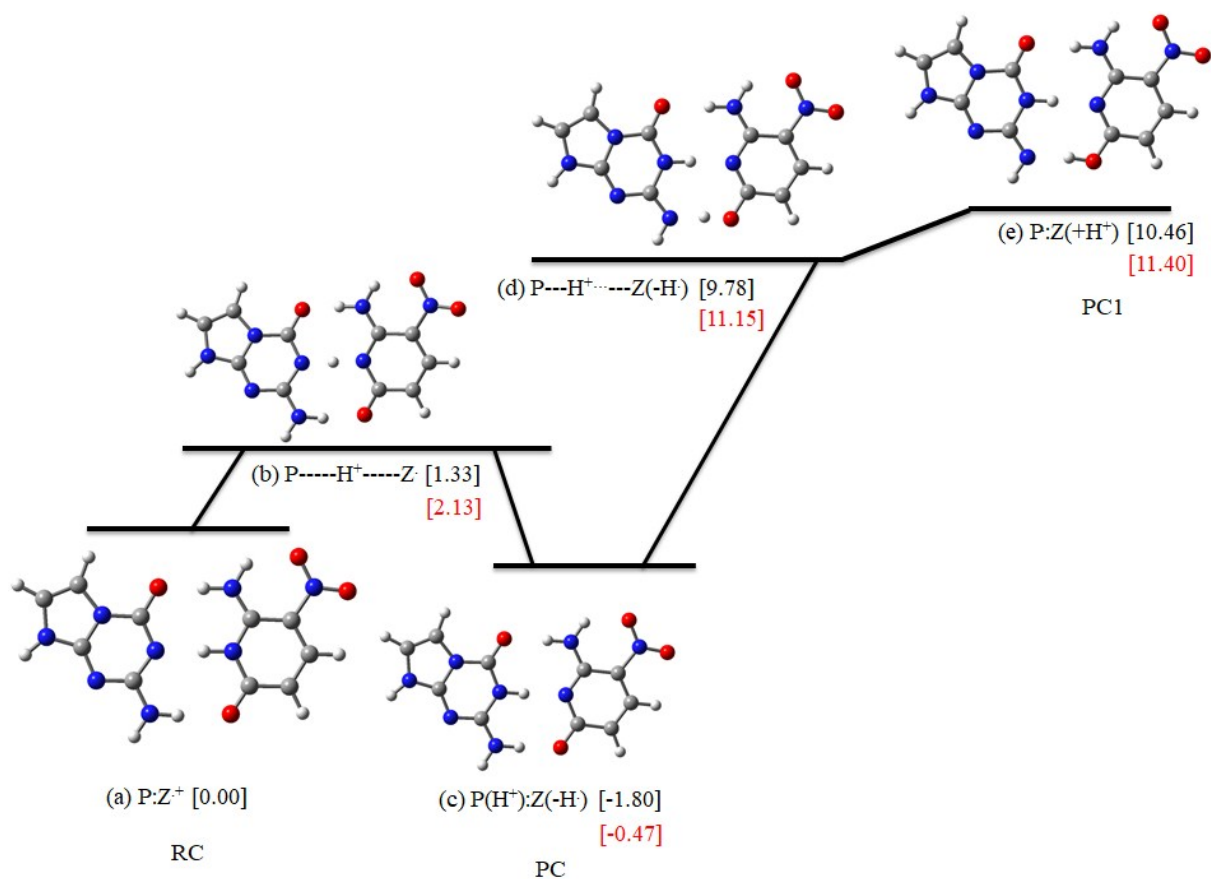


Fig. S2: Potential energy surface of the proton transfer reactions in the $P:Z^+$ complex. The relative ZPE-corrected barrier energies and thermal energy-corrected Gibbs free energies (in red) are also shown.

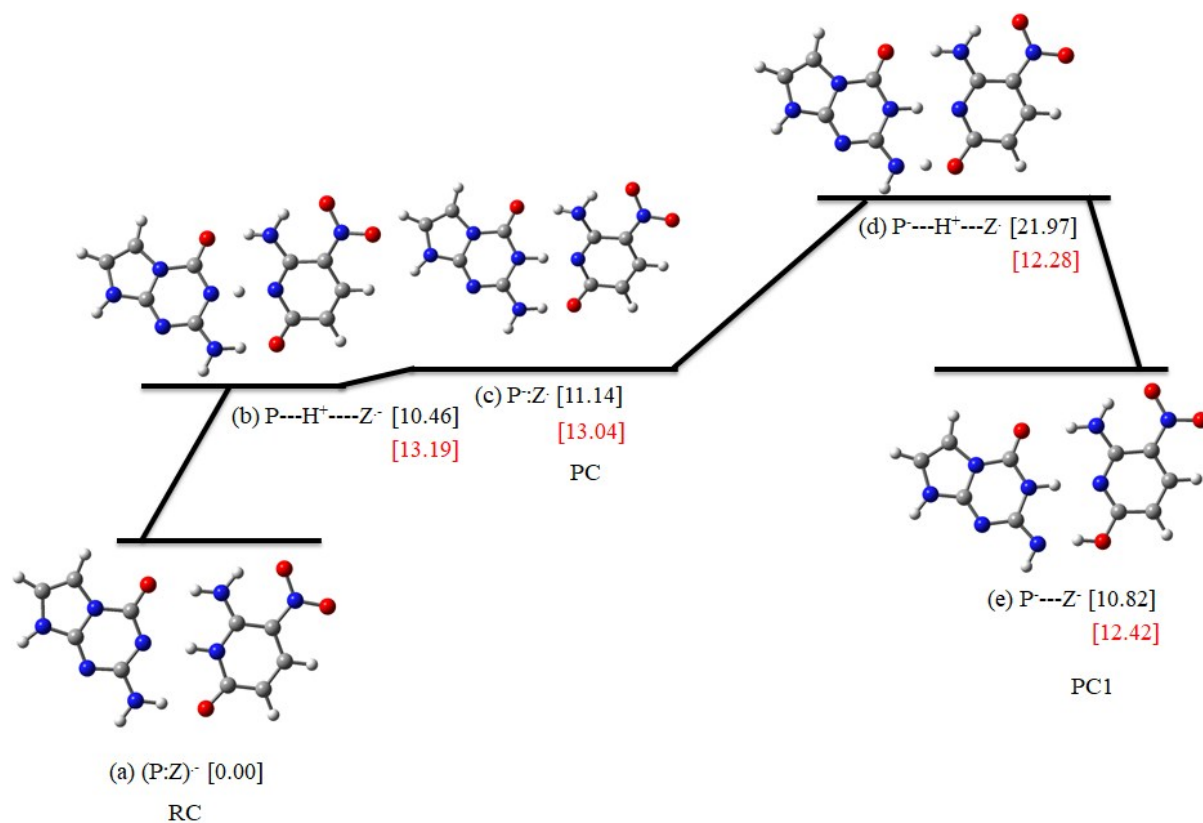


Fig. S3: Potential energy surface of the proton transfer reactions in the $P:Z^-$ complex. The relative ZPE-corrected barrier energies and thermal energy-corrected Gibbs free energies (in red) are also shown.