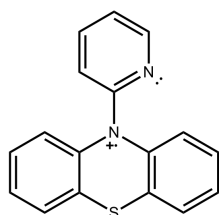


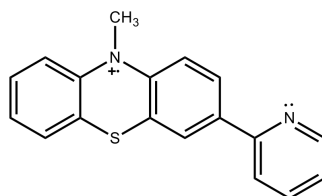
## Determining Transition State Structures for a Series of Concerted Proton-Electron Transfer Agents

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This project has studied hydrogen transfer to two novel, base-appended radical cations: 10-(2-pyridyl)-10*H*-phenothiazinium (PPT) and 3-(2-pyridyl)-10-methylphenothiazium (MPT-pyr). Our recent studies have focused on these molecules abstracting a hydrogen atom from phenol and substituted phenols. Transition states for hydrogen atom transfer have been located using the B972/6-31+g(d,p) model chemistry. We have performed forward and reverse IRC calculations to verify the located transition states connected the proper products and reactants. We have found the forward barrier for hydrogen-atom transfer to be 5-15 kcal/mol, in good agreement with experimental work that has been performed in parallel, albeit always underestimating the barrier height. Our calculated pseudo-first order rate constants of  $100 - 1 \times 10^7 \text{ s}^{-1}$  for hydrogen-atom transfer are also in qualitative agreement with experiment. The low barrier heights and large rate constants for these systems are partially explained by the formation of pre- and post-reaction hydrogen-bonded complexes between the reactants. We have also performed static solvation calculations on the systems, and found that these calculations overestimate the barrier height relative to experimental values.



**PPT**



**MPT-pyr**