

Electronic Supplementary Information

Dipicrylamine as Colorimetric Sensor for Anions: Experimental and Computational Study

Ravi Gunupuru, Manoj K. Kesharwani, Ashish Chakraborty, Bishwajit Ganguly*,
Parimal Paul*

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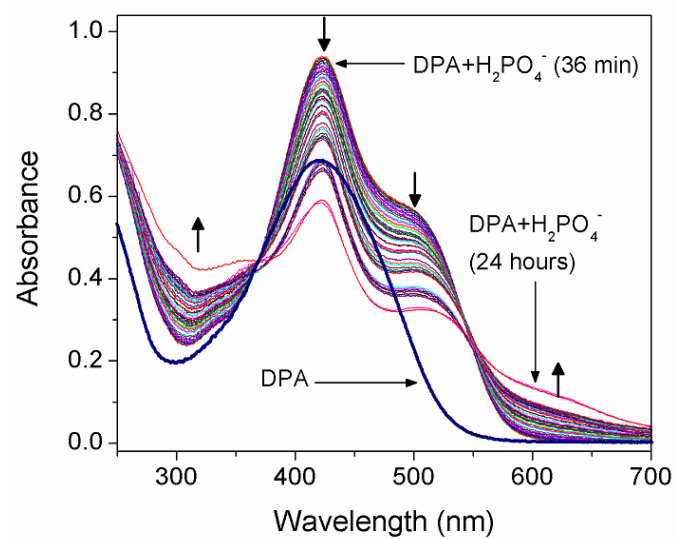


Fig. S1 UV-vis spectral change of DPA in acetonitrile (2.5x10⁻⁵M) as a function of time after addition of TBA(H₂PO₄) (2.5x10⁻³M).

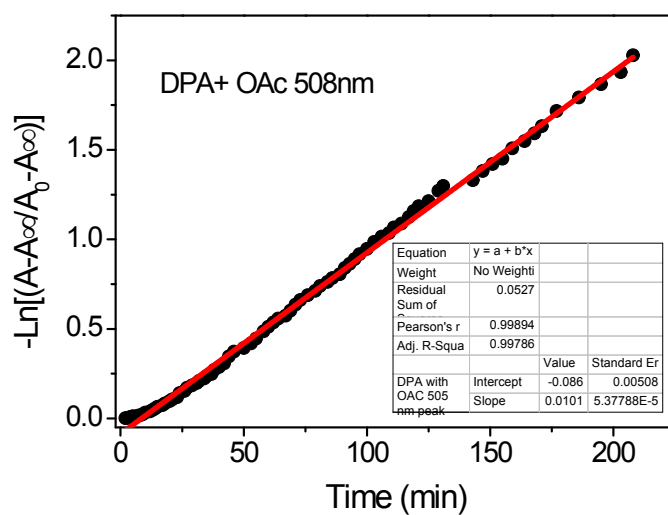


Fig. S2 Plot of the first order rate equation to determine observed rate constant from UV-vis spectral change of DPA as a function of time after addition of TBA(OAc).

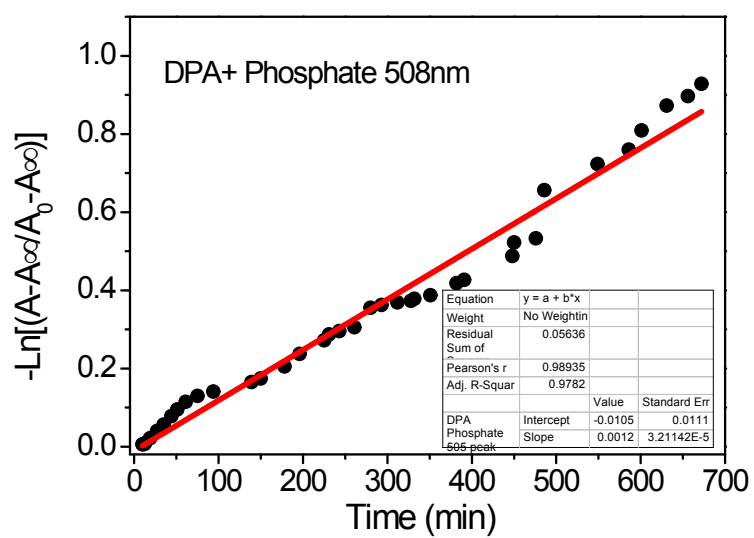


Fig. S3 Plot of the first order rate equation to determine observed rate constant from UV-vis spectral change of DPA as a function of time after addition of TBA(H_2PO_4).

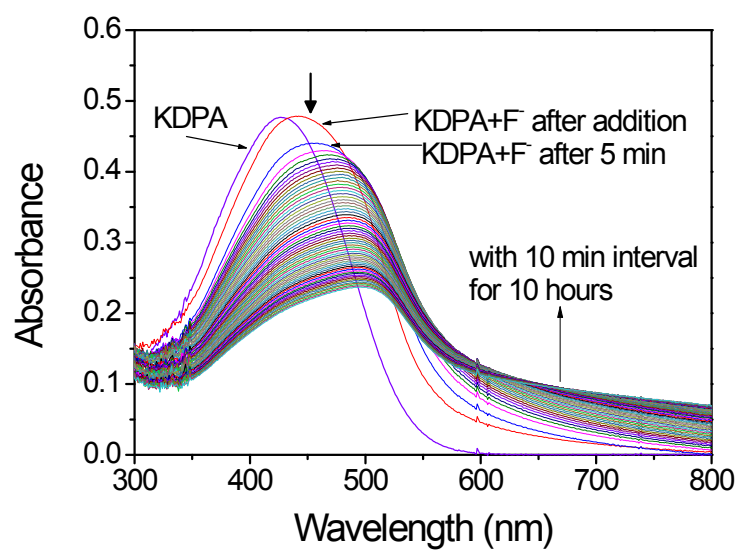


Fig. S4 UV-vis spectra of KDPA in water before and after addition of TBAF.

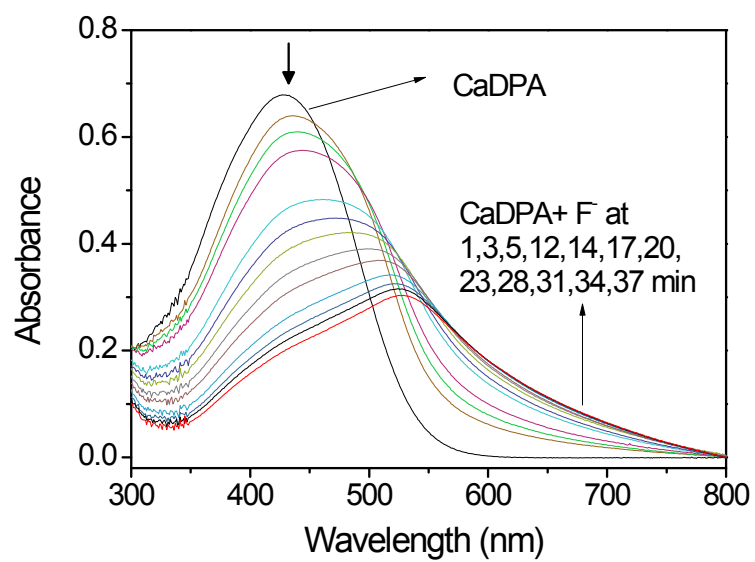


Fig. S5 UV-vis spectra of Ca(DPA)_2 in water before and after addition of TBAF.

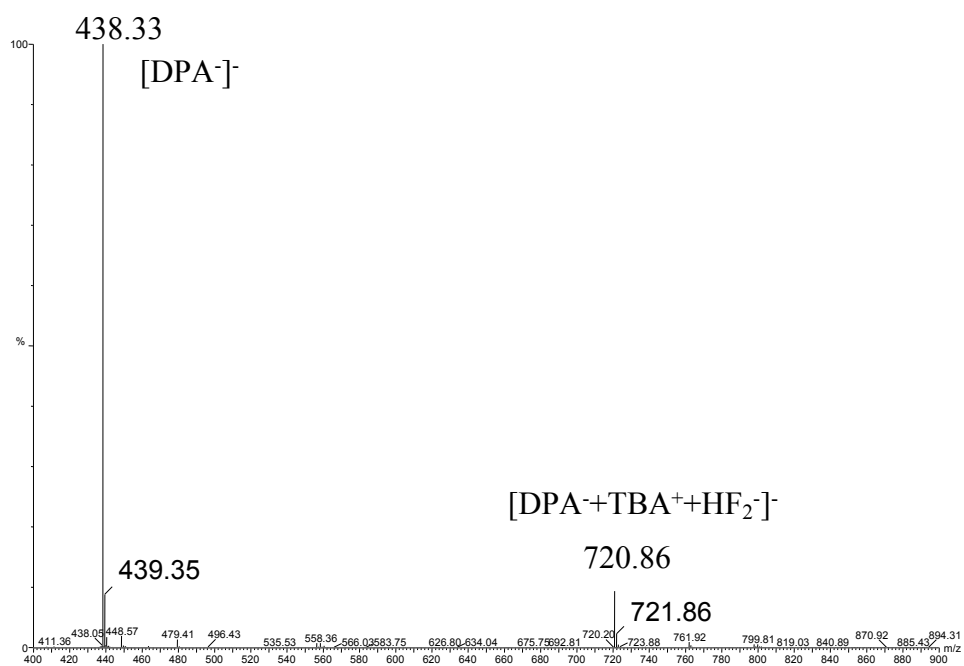


Fig. S6 ES mass spectrum of DPA in acetonitrile after addition of TBAF.

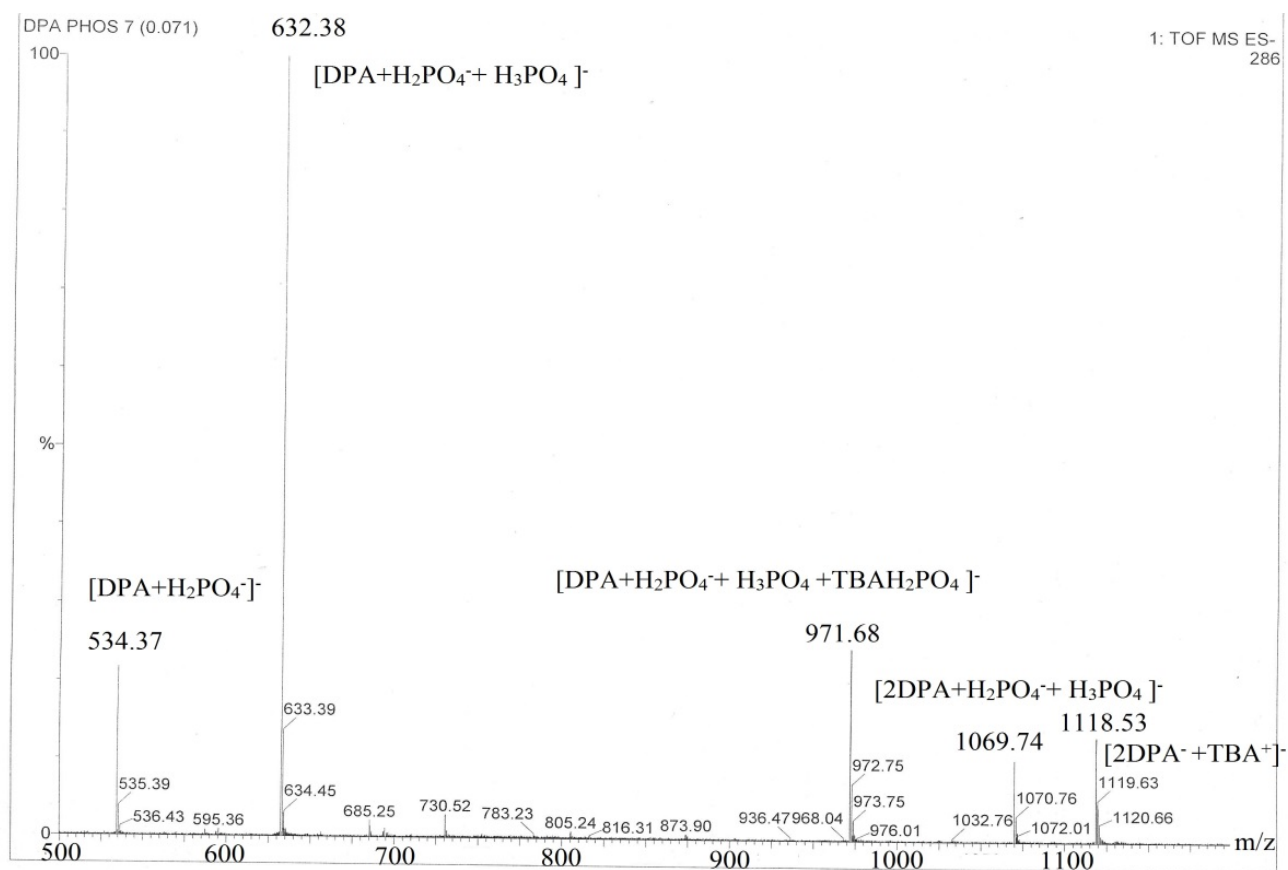


Fig. S7. ES mass spectrum of DPA in acetonitrile after addition of TBA(H_2PO_4).

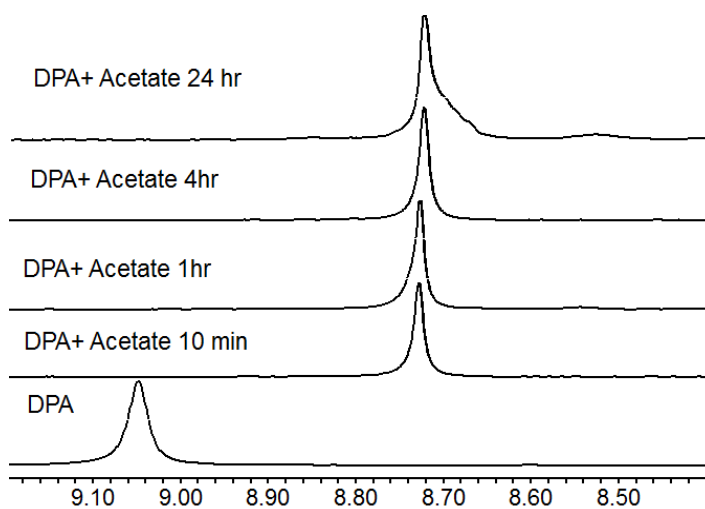


Fig. S8. ^1H NMR spectral change of DPA after addition of TBA(OAc) in CD_3CN .

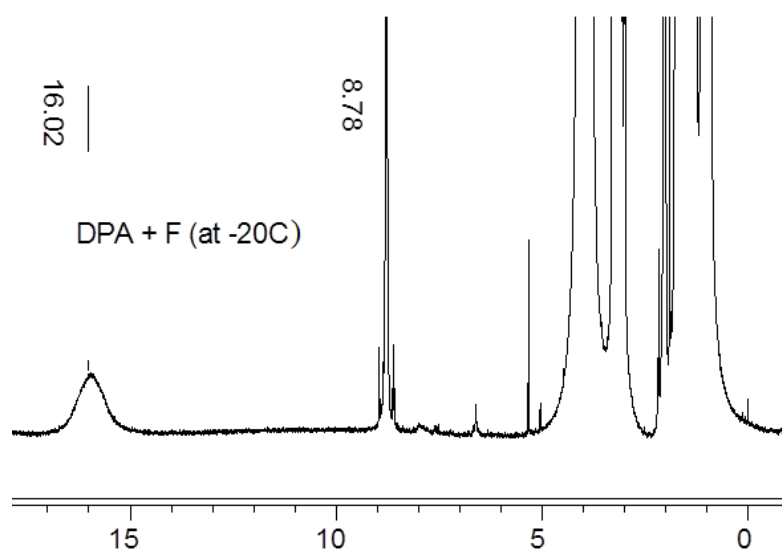


Fig. S9. ^1H NMR spectrum of DPA in acetonitrile at $-20\text{ }^\circ\text{C}$ after addition of TBAF, the signal at 16.02 is due to FHF^- .

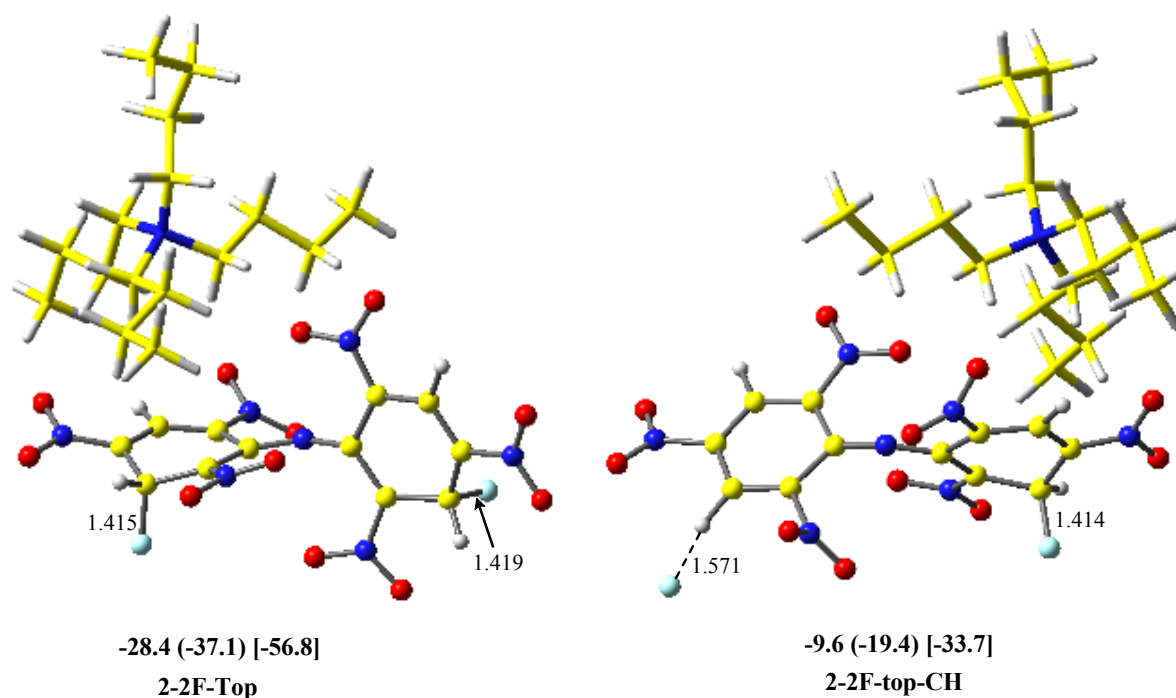


Fig. S10. RHF/6-31+G* optimized geometries, calculated fluoride ion affinities (kcal/mol) and important distances (Å). B3LYP/6-31+G**//RHF/6-31+G* and M06/6-31+G**//RHF/6-31+G* calculated fluoride ion affinities are given in parentheses and square brackets respectively. (yellow = carbon; blue = nitrogen; red = oxygen; white = hydrogen; cyan = fluoride).