

Supporting information

Rapid Colorimetric Discrimination of Cyanide Ions – Mechanistic Insights and Applications

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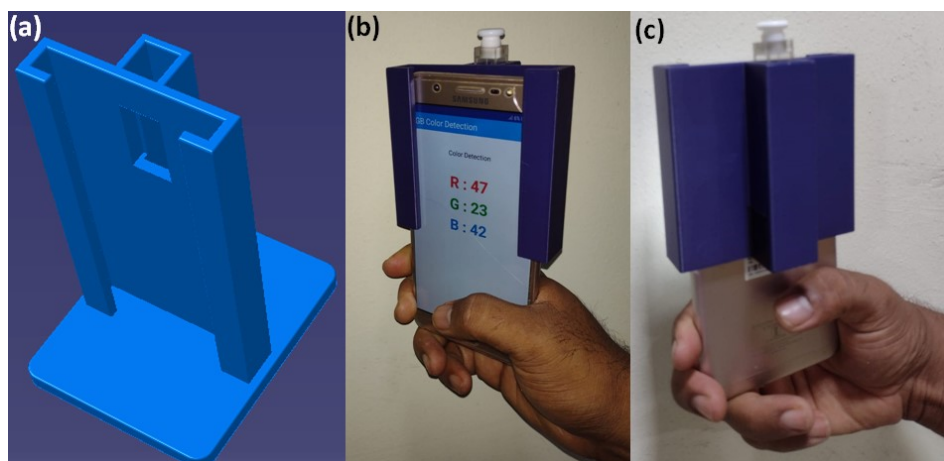
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Table S1: Computed λ_{max} values with different functional and basis set for DMN probe. The experimental λ_{max} value is 645 nm.

Functional	Basis set	λ_{max} (nm)
B3LYP	6-31G	663
	6-31+G	681
	6-31+G*	622
	6-311G	661
	6-311+G	673
BP86	6-31G	874
CAM-B3LYP	6-311G	618
M06-2X	6-31G	635
B3P86	6-31G	740
PBE	6-31G	870



Scheme S1: 3D printed portable module (a) exploded view, (b) front and (c) back view of the 3D module mounted on a smartphone.

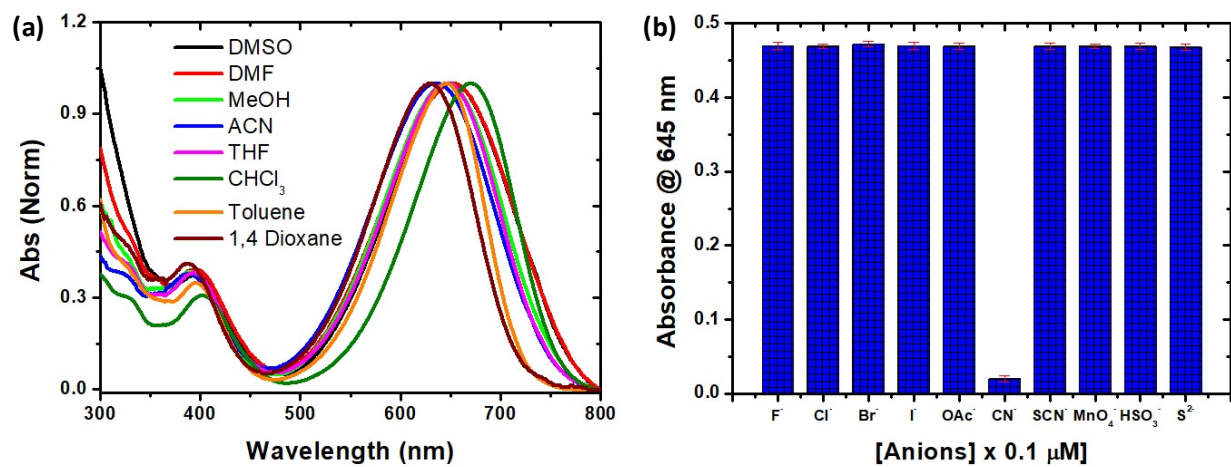


Figure S1: (a) absorption spectrum of DMN in various solvents, (b) selectivity of DMN probe with various analytes.

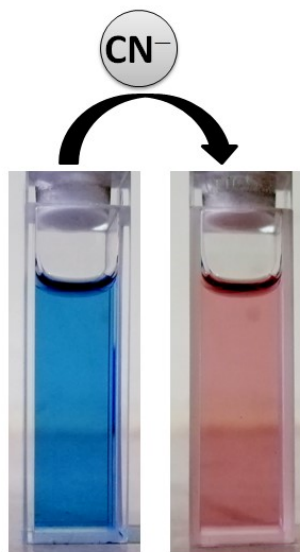


Figure S2: Colorimetric change of DMN probe in the presence of cyanide ions.

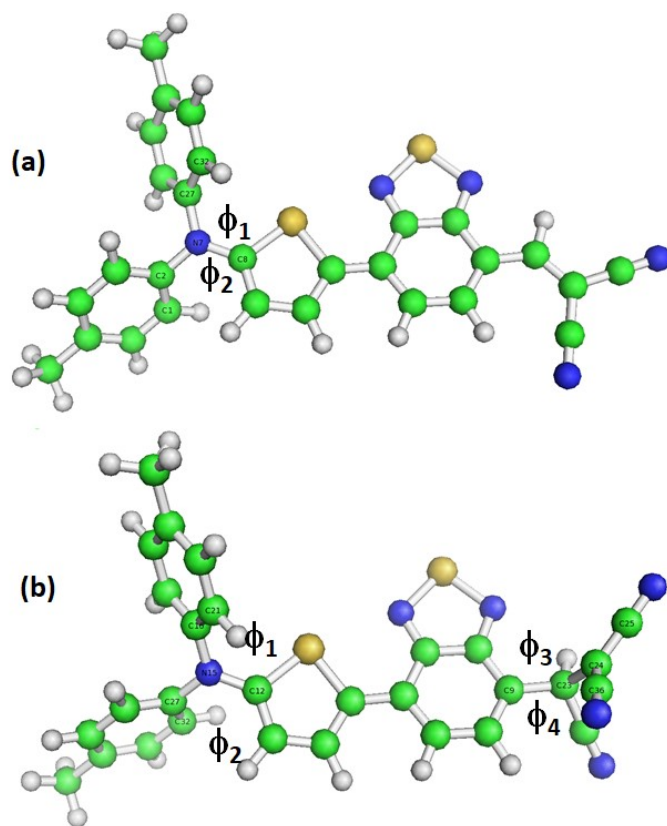


Figure S3: The geometry optimized structures of (a) DMN and (b) with CN.