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A Comprehensive Review on Dicyanoisophorone-Based Donor-π-acceptor Chromophores for Sensing, Bioimaging, and Optoelectronic Applications

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Abstract: Dicyanoisophorone (DCI) and its amino-functionalized derivative dicyanoisophorone amine (DCI-NH_2) represent an important class of donor-π-acceptor (D-π-A) chromophores with exceptional photophysical properties. Owing to strong intramolecular charge transfer (ICT), extended π-conjugation, and tunable electronic structures, these fluorophores exhibit red-shifted absorption, near-infrared (NIR) emission, large Stokes shifts, and pronounced solvatochromism. Such attributes have enabled their widespread use in chemical sensing, biological imaging, optoelectronics, and energy conversion technologies. This review systematically summarizes the structural features, synthetic accessibility, photophysical behavior, and multifunctional applications of DCI and DCI-NH_2 derivatives, with particular emphasis on solvatochromism, environment-sensitive fluorescence, and their roles as NIR probes for bioimaging and sensing.

Keywords*:* Dicyanoisophorone, DCI-NH_2, donor-π-acceptor ,intramolecular charge transfer, solvatochromism, NIR fluorescence, bioimaging

I. INTRODUCTION

Push-pull chromophores based on donor-π-acceptor (D-π-A) architectures have attracted sustained attention due to their unique optical and electronic properties, including strong intramolecular charge transfer (ICT), bathochromic shifts, solvatochromism, and nonlinear optical (NLO) responses [1]. Among these systems, dicyanoisophorone (DCI) has emerged as a versatile scaffold for the development of small-molecule fluorophores, particularly those emitting in the visible to near-infrared (NIR) region [2,3]. The incorporation of strong electron-withdrawing cyano groups and electron-donating substituents enables precise tuning of absorption and emission properties, rendering DCI derivatives highly attractive for applications in sensing, imaging, and optoelectronics.

II. DICYANOISOPHORONE (DCI): STRUCTURE AND PHOTOPHYSICAL PROPERTIES

Dicyanoisophorone (DCI), also referred to as dicyanomethyleneisophorone, is a classical D-π-Achromophore in which a dicyanomethylene acceptor is conjugated to a modified isophorone donor unit through an extended π-system. This planar conjugated backbone facilitates efficient ICT and extensive π-electron delocalization, resulting in high molar extinction coefficients and red-shifted absorption maxima [2].

The strong electron-withdrawing nature of the cyano (-CN) groups stabilizes the lowest unoccupied molecular orbital (LUMO), while the electron-rich isophorone moiety raises the highest occupied molecular orbital (HOMO). This electronic configuration reduces the bandgap and enhances molecular polarizability, leading to intense fluorescence emission spanning the visible to NIR region [4,5].

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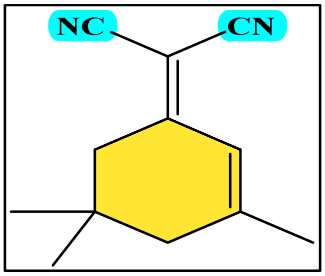

Figure 1.1 Structure of Dicyanoisophorone (DCI)

III. SOLVATOCHROMISM AND INTRAMOLECULAR CHARGE TRANSFER

One of the most notable characteristics of DCI derivatives is their pronounced solvatochromic behavior. Due to strong ICT, both absorption and emission spectra undergo significant red shifts with increasing solvent polarity. In polar environments, the excited state characterized by a higher dipole moment is preferentially stabilized through dipole-dipole interactions and dielectric effects, resulting in bathochromic shifts in fluorescence emission [4,6].Quantitative analysis using Lippert-Mataga plots has demonstrated that DCI-based chromophores can exhibit emission shifts exceeding 100 nm between nonpolar and polar solvents [1,3]. This high environmental sensitivity makes DCI derivatives powerful probes for polarity mapping in micelles, lipid bilayers, polymer matrices, and complex biological systems.

IV. SYNTHETIC ACCESSIBILITY AND STRUCTURAL MODIFICATIONS

A key advantage of DCI lies in its straightforward synthesis and structural versatility. Typically, DCI is synthesized via Knoevenagel condensation between isophorone (or its analogues) and malononitrile, yielding the dicyanomethylene intermediate [2]. Subsequent functionalization at the isophorone ring or along the conjugated arms allows the introduction of diverse donor or acceptor substituents.Such modifications have enabled the development of Schiff base, azo, hydrazone, arylated, and heterocycle-linked DCI derivatives, each tailored for specific photophysical or sensing applications. This modularity facilitates systematic structure-property relationship studies essential for rational probe design.

V. APPLICATIONS OF DCI-BASED CHROMOPHORES

5.1 Chemical and Biological Sensing:

DCI derivatives have been extensively explored as fluorescent sensors for ions, small molecules, and reactive species. Changes in ICT efficiency upon analyte binding often result in fluorescence turn-on/off or ratiometric responses. Notably, DCI-based probes have been reported for the detection of anions (CN^- , F^-), metal ions (Fe^{3+} , Cu^{2+}), reactive oxygen species (ROS), and thiols[3,7,8].

5.2 Bioimaging

The strong NIR emission, large Stokes shifts, and low background autofluorescence of DCI derivatives enable deep tissue penetration and high-contrast imaging. These features have been successfully exploited in live-cell imaging, zebrafish models, and in vivo studies [5,8,9].

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5.3 Optoelectronics and Energy Applications

Beyond sensing, DCI derivatives have been incorporated into organic light-emitting diodes (OLEDs), dye-sensitized solar cells (DSSCs), and organic photovoltaics (OPVs). Their broad absorption profiles and efficient charge transfer characteristics contribute to improved light-harvesting and power conversion efficiencies [5,10].

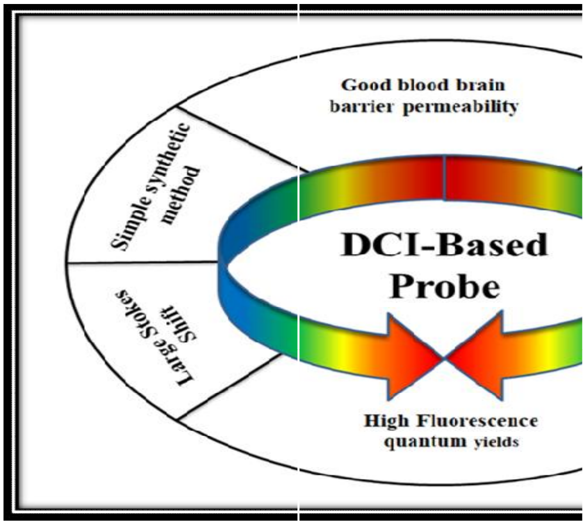

Figure 1.2 Multifunctional attributes of DCI-based probes

VI. DICYANOISOPHORONE AMINE (DCI-NH$_2$): ENHANCED DONOR-Π-ACCEPTOR SYSTEMS

Dicyanoisophorone amine (DCI-NH$_2$) represents a prominent subclass of DCI derivatives in which an electron-donating amino group is introduced at the donor site. This modification significantly enhances ICT strength, solvatochromism, fluorescence quantum yield, and NIR emission [9,11].

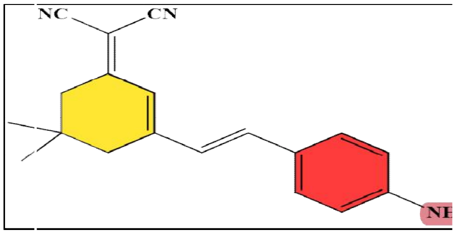

Figure 1.3 Structure of Dicyanoisophorone Amine (DCI-NH□)

The amino substituent increases electron density on the donor moiety, further narrowing the HOMO-LUMO gap and improving environmental sensitivity. Consequently, DCI-NH□ derivatives are particularly suited for ratiometric and turn-on fluorescent probes.

VII. SENSING AND BIOIMAGING APPLICATIONS OF DCI-NH$_2$

DCI-NH$_2$-based probes have been widely applied for the selective detection of biothiols, reactive sulfur/nitrogen species, metal ions, and gasotransmitters such as CO and H_2S [12–15]. Their NIR emission ensures minimal photodamage and deep tissue imaging capability. Recent studies have demonstrated DCI-NH$_2$-based theranostic systems, including inflammatory-stimuli-responsive prodrugs capable of simultaneous imaging and drug delivery [16]. Structural modifications such as aldehyde, chloro, phosphinate, sulfonate, and chelating group incorporation have further improved selectivity, aqueous solubility, and biocompatibility [13–15,17,18].

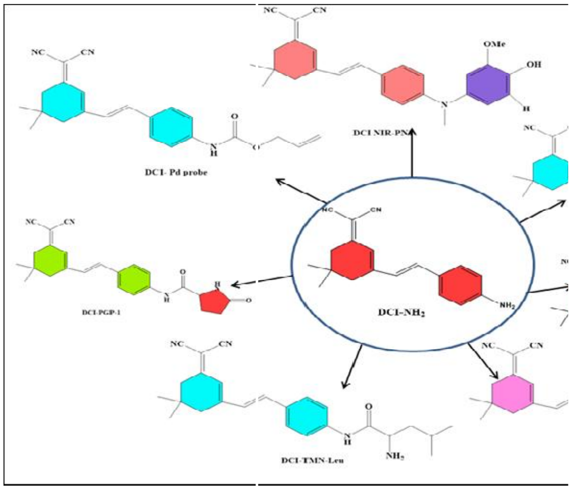

Figure 1.4 Structural modification of the DCI-NH$_2$ scaffold for functional probe development

VIII. CONCLUSIONS AND FUTURE PERSPECTIVES

Dicyanoisophorone and its amino derivatives constitute a robust and versatile class of D-π-Afluorophores with exceptional photophysical properties. Their strong ICT character, pronounced solvatochromism, NIR emission, and synthetic tunability have enabled broad applications across chemical sensing, bioimaging, optoelectronics, and energy conversion. Future research efforts focusing on improving water solubility, targeting specificity, and multimodal sensing capabilities are expected to further expand the utility of DCI and DCI-NH$_2$-based materials in interdisciplinary scientific and technological domains.

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Credit Authorship Contributions Statement

Kajal R. Gaikwad: Conceptualization, , writing-original draft preparation.
Pramod B. Thakur: Supervision, project administration, methodology guidance, writing review, and editing.

Declaration of Competing Interest

The author declares no conflict of interest, whether financial or personal, that could have influenced the reported work.

Consent to Publish Declaration

Not applicable.

Ethics and Consent to Participate Declarations

Not applicable.

Data Availability

The datasets supporting the conclusions of this study can be obtained from the corresponding author on reasonable request.

REFERENCES

[1] Zhao, J., Wu, W., Sun, J., and Guo, S., 2013, "Triplet Photosensitizers: From Molecular Design to Applications," Chem. Soc. Rev., **42**(12), pp. 5323–5351.

[2] Zhang, X., and Chen, Y., 2013, "Synthesis and Fluorescence of Dicyanoisophorone Derivatives," Dye. Pigment., **99**(3), pp. 531–536.

[3] Yan, L., Tang, L., Wu, X., and Li, L., 2024, "Recent Advances in Organic Small-Molecule Fluorescent Probes Based on Dicyanoisophorone Derivatives," Crit. Rev. Anal. Chem., pp. 1–28.

[4] Thomas, D., Rubio, V., Iragavarapu, V., Guzman, E., Pelletier, O. B., Alamgir, S., Zhang, Q., and Stawikowski, M. J., 2021, "Solvatochromic and PH-Sensitive Fluorescent Membrane Probes for Imaging of Live Cells," ACS Chem. Neurosci., **12**(4), pp. 719–734.

[5] Dai, L., Zhang, Q., Ma, Q., and Lin, W., 2023, "Emerging near Infrared Fluorophore: Dicyanoisophorone-Based Small-Molecule Fluorescent Probes with Large Stokes Shifts for Bioimaging," Coord. Chem. Rev., **489**, p. 215193.

[6] Ma, J., Sun, R., Xia, K., Xia, Q., Liu, Y., and Zhang, X., 2024, "Design and Application of Fluorescent Probes to Detect Cellular Physical Microenvironments," Chem. Rev., **124**(4), pp. 1738–1861.

[7] Jia, J., Xue, P., Zhang, Y., Xu, Q., Zhang, G., Huang, T., Zhang, H., and Lu, R., 2014, "Fluorescent Sensor Based on Dimesitylborylthiophene Derivative for Probing Fluoride and Cyanide," Tetrahedron, **70**(35), pp. 5499–5504.

[8] Liu, F.-T., Han, W.-W., Ren, H., Wang, R.-N., Yang, W.-J., Miao, J.-Y., Zhao, B.-X., and Lin, Z.-M., 2023, "A Dicyanoisophorone-Quinolinium-Based near-Infrared-Emission Fluorescent Probe for Ratiometric Sensing of Bisulfite/Sulfite in Living Cells," Sensors Actuators B Chem., **380**, p. 133305.

[9] Zhao, Y., Wei, K., Kong, F., Gao, X., Xu, K., and Tang, B., 2019, "Dicyanoisophorone-Based Near-Infrared-Emission Fluorescent Probe for Detecting NAD(P)H in Living Cells and in Vivo," Anal. Chem., **91**(2), pp. 1368–1374. https://doi.org/10.1021/acs.analchem.8b03563.

[10] Kumar, A., 2024, "Recent Development in Fluorescent Probes for the Detection of Hg2+ Ions," Crit. Rev. Anal. Chem., **54**(8), pp. 3269–3312.

[11] Chakraborty, S., Paul, S., Roy, P., and Rayalu, S., 2021, "Detection of Cyanide Ion by Chemosensing and Fluorosensing Technology," Inorg. Chem. Commun., **128**, p. 108562.

[12] Hou, J., Cai, P., Wang, C., and Shen, Y., 2018, "A Novel Fluorescent Probe with a Large Stokes Shift for Cysteine Based on Dicyanoisophorone," Tetrahedron Lett., **59**(26), pp. 2581–2585.

[13] Jia, P., Liu, D., Zhuang, Z., Liu, C., Li, Z., Yu, C., Chen, Y., Zhu, H., Zhang, X., and Yu, Y., 2019, "Dicyanoisophorone-Derived near-Infrared Fluorescent Probe for Ultrasensitive Detection of Peroxynitrite in Living Cells and Zebrafish," Ind. Eng. Chem. Res., **58**(43), pp. 19778–19784.

[14] Hong, J., Feng, W., and Feng, G., 2018, "Highly Selective Near-Infrared Fluorescent Probe with Rapid Response, Remarkable Large Stokes Shift and Bright Fluorescence for H2S Detection in Living Cells and Animals," Sensors Actuators B Chem., **262**, pp. 837–844.

[15] Wang, J., Wen, Y., Huo, F., and Yin, C., 2019, "A Highly Sensitive Fluorescent Probe for Hydrogen Sulfide Based on Dicyanoisophorone and Its Imaging in Living Cells," Sensors Actuators B Chem., **294**, pp. 141–147.

[16] Sufian, A., Parihar, N., Badirujjaman, M., Barman, P., Kesarwani, R., Pemmaraju, D. B., and Bhabak, K. P., 2024, "Inflammatory-Stimuli-Responsive Turn-on NIR Fluorogenic Theranostic Prodrug: Adjuvant

DOI: 10.48175/IJARSCT-31734

Delivery of Diclofenac and Hydrogen Sulfide Attenuates Acute Inflammatory Disorders," J. Mater. Chem. B, **12**(17), pp. 4248–4261.

[17] Liu, B., Zhao, X., Zhou, M., Song, C., Zeng, C., Qin, T., Zhang, M., and Xu, Z., 2022, "Modulating Donor of Dicyanoisophorone-Based Fluorophores to Detect Human Serum Albumin with NIR Fluorescence," Spectrochim. Acta Part A Mol. Biomol. Spectrosc., **268**, p. 120666.

[18] Peng, Z., Li, Z., Zhou, T., Wu, D., Wang, E., Ma, C., Lu, C., Nie, J., Fan, G., and Yang, G., 2023, "Visualizing Biothiols in Vivo Using a Dual-Channel Sensitive Fluorescent Probe," Dye. Pigment., **214**, p. 111230.

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