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Synthesis, crystal structure and spectral properties of 2-[(1-Methyl-2-benzimidazolyl)azo]-p-cresol: An experimental and theoretical study

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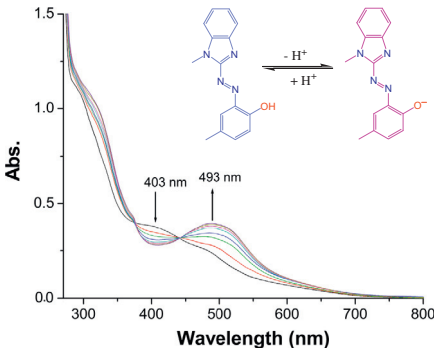
HIGHLIGHTS

- Azophenol ligand containing benzimidazole moiety.
- X-ray crystal structure.
- Electronic structure and photophysical property.
- DFT and TDDFT calculation.

GRAPHICAL ABSTRACT

2-[(1-Methyl-2-benzimidazolyl)azo]-p-cresol (HL), containing phenolic-OH function and benzimidazole moiety has been synthesized and characterized. The chemical, electronic structure and photophysical properties have been studied by spectroscopic analysis abetted with DFT and TDDFT calculations. The change in electronic spectra of HL by titration with aq. NaOH is studied and well supported by TDDFT calculations. The molecule forms 2D-supramolecular structure by inter-molecular H-bonding and π–π interactions.



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ABSTRACT

2-[(1-Methyl-2-benzimidazolyl)azo]-p-cresol (HL), containing phenolic-OH function and benzimidazole moiety has been synthesized and characterized. The chemical, electronic structure and photophysical properties have been studied by spectroscopic analysis abetted with DFT and TDDFT calculations. The change in electronic spectra of HL by titration with aq. NaOH is studied and well supported by TDDFT calculations. The structure is confirmed by single crystal X-ray study. In the unit cell, two HL molecules are H-bonded with H_2O molecule and forms dimmeric structure. The molecule forms 2D-supramolecular structure by inter-molecular H-bonding and π–π interactions.

Introduction

Benzimidazoles are very useful intermediates for the development of molecules of biological interest. Benzimidazole and its derivative have found applications in biological activities such as

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antimicrobial, anticancer, anti-inflammatory, antivirus and anti-convulsant [1–10]. Benzimidazole based ligands can be used to prepare luminescent metal complexes and form supramolecular architectures. Planar benzimidazole based ligands can engage in π–π stacking interactions and have also shown LMCT charge transfer properties in the complexes [11–14].

Proton transport in bio-molecules is of utmost importance for bioenergetics [15,16]. This stimulates high research activity in the field of proton-transfer dynamics in organic molecules [17–19]. Aromatic weak acids and bases have found use as proton-transfer fluorescent probes for surfactants and macromolecules [18,20,21]. Such probes have been utilized by several groups to elucidate the effects of microenvironment on the equilibrium and rate constants of the excited-state proton transfer in micelles, liposomes, microemulsions and LB films [22–27]. Effects of the surface potential on apparent p*K* and protolytic photodissociation rate constants, correlation between rate constants and apparent p*K* in micelles of different charge, and kinetic nonequivalence of proton-transfer probes in liposomes have been revealed [22,28–30].

The present work describes the synthesis and characterizations of 2-[(1-Methyl-2-benzimidazolyl)azo]-p-cresol (HL), containing phenolic-OH function and benzimidazole moiety. The chemical, electronic structure and photophysical properties have been studied by spectroscopic analysis abetted with DFT and TDDFT calculations.

Experimental

Material and methods

2-Amino-4-methylphenol and benzimidazole were purchased from Aldrich. All other organic chemicals and inorganic salts were available from Sisco Research Lab, Mumbai, India and used without further purification. Commercially available SRL silica gel (60–120 mesh) was used for column chromatography.

Microanalytical data (C, H, N) were collected on Perkin–Elmer 2400 CHNS/O elemental analyzer. ESI mass spectra were recorded on a micromass Q-TOF mass spectrometer. Infrared spectra were taken on a RX-1 Perkin Elmer spectrophotometer with samples prepared as KBr pellets. Electronic spectral studies were performed on a Perkin Elmer Lambda 25 spectrophotometer. NMR spectra were recorded using a Bruker (AC) 300 MHz FTNMR spectrometer in $CDCl_3$. The pH of the solutions was measured on a Systronics μpH System 361. Triply distilled water was used wherever required.

Synthesis of 2-[(1-Methyl-2-benzimidazolyl)azo]-p-cresol (HL)

2-Amino-4-methylphenol (4.0 g, 32.4 mmol) was dissolved in 5 mL conc. HCl and 10 mL distilled water and cooled to 0 °C. Sodium nitrite (2.8 g, 42.12 mmol) was dissolved in minimum volume of water and cooled to 0 °C. The diazotized solution was added dropwise with constant stirring to benzimidazole (4.0 g, 34.0 mmol) dissolved in aqueous solution of sodium carbonate (5.1 g, 48.0 mmol). The product was purified by column chromatography using silica gel (60–120 mesh) and eluted by 20% (v/v) ethyl acetate petroleum ether mixture. Yield was, 5.1 g 64%.

3.2 g (12.6 mmol) of the diazo-coupled product was taken and N-methylation was performed with MeI (1.8 g, 13.0 mmol) using NaH (1.0 g, 25.1 mmol) as base in dry THF medium following the reported methods [31]. The product was subjected to chromatographic separation on a silica gel column (60–120 mesh). The desired red band of HL was eluted with 10% (v/v) ethyl acetate petroleum ether mixture. Evaporation of the solvent under reduced pressure afforded pure compound. Yield was 2.1 g, 62%.

Table 1
Crystallographic data and refinement parameters for HL.

Empirical formula	$C_{30}H_{30}N_8O_3$
Moiety formula	$2(C_{15}H_{14}N_4O)$, H_2O
Formula weight	533.99
Crystal system	Triclinic
Space group	$P-1$
a (Å)	8.590(5)
b (Å)	11.789(5)
c (Å)	14.670(5)
α (°)	76.674(5)
β (°)	86.065(5)
γ (°)	88.027(5)
V (Å^3)	1441.9(11)
Z	2
ρ_{calcd} (g cm^3)	1.268
μ (mm^{-1})	0.086
T (K)	293(2)
hkl range	−10 to 10, −14 to 14, −17 to 17
$F(000)$	580
θ range (°)	1.78–25.99
Reflns collected	13,930
Unique reflns (R_{int})	5600 [0.0622]
Observed data ($I > 2\sigma(I)$)	2030
Data/restraints/parameters	5600/0/372
R_1[a], wR_2[b] ($I > 2\sigma(I)$)	0.0641, 0.1182
R_1, wR_2 (all data)	0.1978, 0.1467
GOF[c]	1.092
Largest diff. peak/hole (e Å^3)	0.237/−0.187

[a] $R_1 = \sum |(|F_o| - |F_c|)| / \sum |F_o|$.

[b] $wR_2 = \sum \left[w\left(F_o^2 - F_c^2\right)^2 \right] / \sum \left[w\left(F_o^2\right)^2 \right]^{1/2}$, $w = 1/\left[\sigma^2\left(F_o^2\right) + (0.0345P)^2 \right]$,

where $P = \left(F_o^2 + 2F_c^2\right)/3$.

[c] $GOF = \sum \left[w\left(F_o^2 - F_c^2\right)^2 \right] / (n-p)^{1/2}$,

where n = number of measured data and p = number of parameters.

Anal. Calc. for $C_{15}H_{14}N_4O$ (HL): C, 67.65; H, 5.30; N, 21.04%. Found: C, 67.82; H, 5.32; N, 21.11%. IR data (KBr, cm^{-1}): 3373 υ(O—H); 1620 υ(C=N); 1419 υ(N=N). ^{1}H NMR data ($CDCl_3$, ppm): 13.45 (1H, s), 7.84 (1H, s), 7.78 (1H, d, J = 7.5 Hz), 7.64 (1H, d, J = 8.0 Hz), 7.37 (1H, d, J = 7.5 Hz), 7.23–7.33 (3H, m), 3.79 (3H, s), 2.14 (3H, s).

Crystallography

Details of crystal analysis, data collection and structure refinement data for HL is given in Table 1. Crystal mounting was done on glass fibers with epoxy cement. Single crystal data collections were performed with an automated Bruker SMART APEX CCD diffractometer using graphite monochromatized Mo Kα radiation (λ = 0.71073 Å). Reflection data were recorded using the ω scan technique. Unit cell parameters were determined from least-squares refinement of setting angles with θ in the range $1.78 \leqslant \theta \leqslant 25.99°$. Out of 13,930 collected data 5600 with $I > 2\sigma(I)$ were used for structure solution. These were in the $-10 \leqslant h \leqslant 10, -14 \leqslant k \leqslant 14, -17 \leqslant l \leqslant 17$. The structures were solved and refined by full-matrix least-squares techniques on F^2 using the SHELXS-97 program [32]. The absorption corrections were done by the multi-scan technique. All data were corrected for Lorentz and polarization effects, and the non-hydrogen atoms were refined anisotropically. Hydrogen atoms were generated using SHELXL-97 [32] and their positions calculated based on the riding mode with thermal parameters equal to 1.2 times that of associated C atoms, and participated in the calculation of the final R-indices.

Computational method

All computations were performed using the Gaussian03 (G03) program [33]. Full geometry optimization of HL and L^- were carried out using the DFT method at the B3LYP level of theory [34,35]. The 6-31+G(d) basis set was assigned for C, H, N and O atoms [36]. The vibrational frequency calculations were performed to ensure that the optimized geometries represent the local minima of potential energy surface and there are only positive eigenvalues. The lowest 40 singlet–singlet vertical electronic excitations based on B3LYP optimized geometries were computed using the time-dependent density functional theory (TDDFT) formalism [37–39] in methanol using conductor-like polarizable continuum model (CPCM) [40–42] with the same B3LYP level and basis sets.

Results and discussion

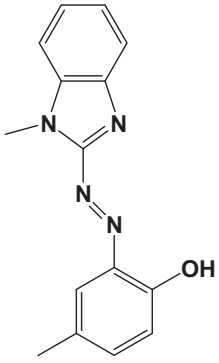
Synthesis and spectral characterization

The titled compound, 2-[(1-Methyl-2-benzimidazolyl)azo]-p-cresol (HL) (Scheme 1) has been synthesized by coupling of diazotized 2-Amino-4-methylphenol with benzimidazole in alkaline medium. The compound has been characterized by elemental and mass spectral analysis along with other spectroscopic techniques (IR, UV–Vis, NMR, etc.) (see Experimental). The structure has been confirmed by X-ray crystal structure analysis.

In the IR spectra, the broad stretching at 3373 cm^{-1} corresponding to υ(OH), the υ(C=N) and υ(N=N) appeared at 1620 and 1419 cm^{-1}. The ^1H NMR spectra of the compound was taken in $CDCl_3$ and the signals appeared as expected. The two sharp singlets at 3.79 and 2.14 ppm correspond to N—Me of the benzimidazole moiety and Me group of p-cresol moiety respectively. The aromatic proton signals appeared at 7.23–7.84 ppm.

Crystal structure

Single crystal suitable for structure determination was obtained by slow diffusion of n-hexane into dichloromethane solution of HL. The crystallographic data collection and refinement parameters are given in Table 1; selected bond lengths are given in Table 2. Molecular structure with atomic numbering scheme is shown in Fig. S1. The bond distances are found as expected, the azo bond length, N(3)—N(4), 1.265(3) Å, C—O bond distance of phenolic group, C(2)—O(1), 1.355(4) Å shows perfect single bond character. In the unit cell, two HL molecules are H-bonded with H_2O molecule and forms dimmeric structure (d(H1···O3, 1.92 Å), d(H2···O3, 1.91 Å), d(H1O3···N6, 2.02 Å) and d(H2O3···N2, 1.92 Å) with ∠D—H···A, 154–175°) (Fig. S2) in addition the intra-molecular H-bonding between phenolic-OH and azo-N (d(H1···N4, 2.28 Å and d(H2···N8, 2.30 Å)) (Table 3). The unit-cell packing diagram is formed due to both inter-molecular H-bonding and π–π (Cg—Cg) interactions between imidazole–imidazole (Cg1—Cg1, 3.588(3) Å and Cg5—Cg5, 3.387(3) Å), imidazole–phenyl (Cg1—Cg2, 3.967(3) Å, Cg1—Cg3, 3.859(3) Å Cg5—Cg6, 4.087(3) Å and Cg5—Cg7, 4.194(3) Å) and phenyl–phenyl (Cg2—Cg2, 4.181(4) Å and Cg2—Cg3, 3.957(3) Å) rings (Fig. S3 and Table 4).



Scheme 1. Structure of 2-[(1-Methyl-2-benzimidazolyl)azo]-p-cresol (HL) ligand.

Electronic spectra and DFT calculation

Electronic spectrum in methanol–water of HL shows a broad peak at 403 nm along with a strong band at 288 nm. The low energy broad band significantly depends on the pH of the medium. Upon titration with aq. NaOH solution the intensity of low energy band is reduced and new bands are generated at 493 nm and 368 nm (Fig. 1).

To get deep insight into the electronic structure and spectra DFT and TDDFT calculations of HL and L^- have been performed. Contour plots of some selected molecular orbitals of HL and L^- are shown in Figs. S4 and S5 respectively. The calculated electronic spectra in

Table 2
Some selected X-ray and calculated bond distances of HL.

Bonds (Å)	X-ray	Calc.
O(1)—C(2)	1.355(4)	1.349
N(1)—C(8)	1.367(4)	1.390
N(1)—C(14)	1.369(4)	1.377
N(2)—C(8)	1.322(4)	1.322
N(2)—C(9)	1.376(4)	1.374
N(3)—C(8)	1.394(4)	1.388
N(3)—N(4)	1.265(3)	1.267
N(4)—C(1)	1.396(4)	1.390
C(1)—C(2)	1.388(4)	1.417
C(1)—C(6)	1.401(4)	1.412
C(2)—C(3)	1.379(5)	1.401
C(3)—C(4)	1.366(4)	1.388
C(4)—C(5)	1.391(5)	1.416
C(5)—C(6)	1.368(5)	1.388
C(9)—C(14)	1.390(5)	1.422

Table 3
Potential intra- and inter-molecular hydrogen bonds in HL.

D—H···A	d (D—H) (Å)	d (H···A) (Å)	d (D···A) (Å)	∠ D—H···A (°)	Type
O1—H1···O3	0.82	1.92	2.740(4)	154	Inter
O1—H1···N4	0.82	2.28	2.719(4)	114	Intra
O3—H1O3···N6	0.86	2.02	2.858(4)	165	Inter
O2—H2···O3	0.82	1.91	2.671(4)	154	Inter
O2—H2···N8	0.82	2.30	2.738(4)	114	Intra
O3—H2O3···N2	0.87	1.92	2.785(4)	175	Inter

Table 4
Inter-molecular Cg—Cg interaction in HL.

Cg—Cg[a]	d (Cg—Cg) (Å)	β (°)[b]	Symmetry
Cg1—Cg1	3.588(3)	14.42	1 − X, 1 − Y, −Z
Cg1—Cg2	3.967(3)	26.95	−X, 1 − Y, −Z
Cg1—Cg3	3.859(3)	26.39	1 − X, 1 − Y, −Z
Cg2—Cg2	4.181(4)	36.06	−X, 2 − Y, −Z
Cg2—Cg3	3.957(3)	22.41	−X, 1 − Y, −Z
Cg5—Cg5	3.387(3)	8.68	−X, 1 − Y, 1 − Z
Cg5—Cg6	4.087(3)	33.48	1 − X, 1 − Y, 1 − Z
Cg5—Cg7	4.194(3)	36.94	1 − X, 2 − Y, 1 − Z

[a] Cg1: N1—C8—N2—C9—C14; Cg2: C1—C2—C3—C4—C5—C6; Cg3: C9—C10—C11—C12—C13—C14; Cg5: N5—C23—N6—C24—C29; Cg6: C16—C17—C18—C19—C20— C21; Cg(7): C24—C25—C26—C27—C28—C29.
[b] β = Angle between the ring.

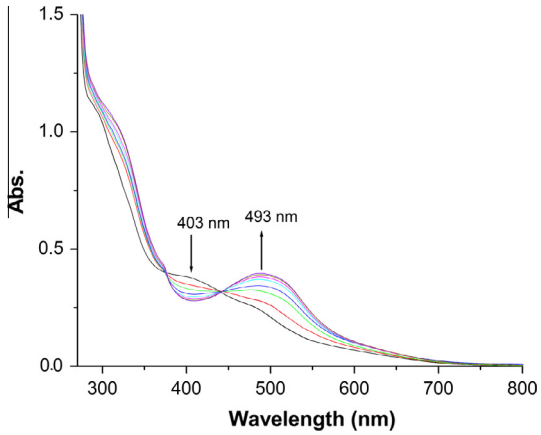


Fig. 1. Change of UV spectrum of HL with addition of aq. NaOH solution (pH = 12).

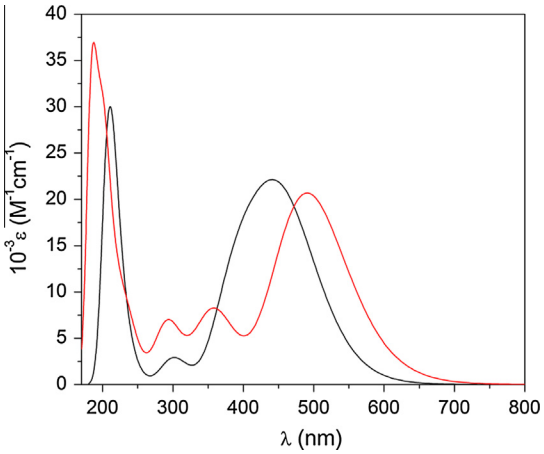


Fig. 2. Theoretical spectra of HL in neutral (––) and anionic (L^-) (____) form.

MeOH are shown in Fig. 2. The transition at 463 nm ($f = 0.0$) corresponding to $n \rightarrow \pi^*$ transition is not well resolved in experimental spectrum of HL. The bands at 403 and 288 nm for HL corresponds to $\pi \rightarrow \pi^*$ transitions (Table 5). For L^- the HOMO → LUMO transition with $f = 0.31$ ($\pi \rightarrow \pi^*$) at 497 nm has been found which is experimentally observed at 493 nm (Table 6). The other experimentally observed bands at 368 and 311 nm also corresponds to

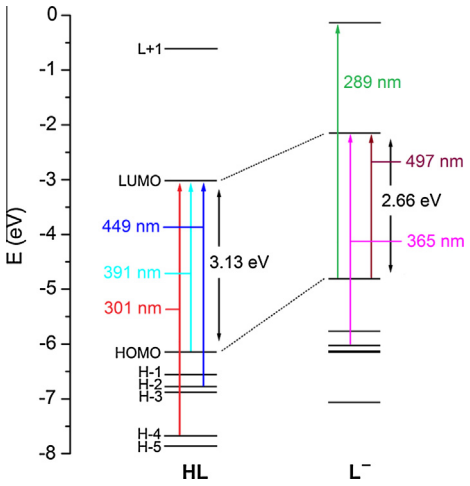


Fig. 3. Energy-level correlation diagram and some selected vertical electronic excitations of HL and L^- calculated by TDDFT/B3LYP method.

$\pi \rightarrow \pi^*$ transitions. The key transitions and the corresponding participated molecular orbitals are shown in co-relation diagram Fig. 3.

Conclusion

2-[(1-Methyl-2-benzimidazolyl)azo]-p-cresol (HL), containing phenolic-OH function and benzimidazole moiety has been synthesized and characterized. The chemical, electronic structure and photophysical properties have been studied by spectroscopic analysis abetted with DFT and TDDFT calculations. The electronic spectra of both HL and L^- obtained by titration with aq. NaOH are well supported by TDDFT results. The structure is confirmed by single crystal X-ray study. The molecule forms 2D-supramolecular structure by inter-molecular H-bonding and π–π interactions.

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Table 5
Vertical electronic excitations calculated by TDDFT/B3LYP/CPCM method of HL in MeOH.

$E_{excitation}$ (eV)	$\lambda_{excitation}$ (nm)	Osc. Strength (f)	Key transitions	Character	λ_{max} (nm)
2.6772	463.1	0.0000	(98%)HOMO−3 → LUMO	$n \rightarrow \pi^*$	
2.7606	449.1	0.3111	(97%)HOMO → LUMO	$\pi \rightarrow \pi^*$	403 (5081)
3.1712	391.0	0.2660	(94%)HOMO−2 → LUMO	$\pi \rightarrow \pi^*$	
4.1169	301.2	0.0862	(92%)HOMO−4 → LUMO	$\pi \rightarrow \pi^*$	288 (18,958)

Table 6
Vertical electronic excitations calculated by TDDFT/B3LYP/CPCM method of L^- in MeOH.

$E_{excitation}$ (eV)	$\lambda_{excitation}$ (nm)	Osc. Strength (f)	Key transitions	Character	λ_{max} (nm)
2.4958	496.8	0.3056	(98%)HOMO → LUMO	$\pi \rightarrow \pi^*$	493
3.4012	364.5	0.1522	(87%)HOMO−2 → LUMO	$\pi \rightarrow \pi^*$	368
3.5855	345.8	0.0396	(90%)HOMO−4 → LUMO	$n \rightarrow \pi^*$	
4.2941	288.7	0.1520	(73%)HOMO → LUMO+1	$\pi \rightarrow \pi^*$	311

Appendix A. Supplementary material

Crystallographic data for the structure HL has been deposited with the Cambridge Crystallographic Data center, CCDC No. 813663. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (e-mail: deposit@ccdc.cam.ac.uk or htpp://www.ccdc.cam.ac.uk). Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.saa.2013.06.049.

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