Effects of Non Covalent Interactions in Light Emitting Properties of \textit{bis}-pyridyl-alkyl-di-imines

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\textbf{General}

Infra-red spectrum was recorded in FTIR ABB Bomen MB-3000. UV-Vis absorption spectra were recorded in Shimadzu Spectrophotometer with model UV-2450. Fluorescence spectra were recorded in Shimadzu Spectrofluorophotometer with model RF-5301PC. \textsuperscript{1}H and \textsuperscript{13}C nuclear magnetic resonance spectra were measured on a 400 MHz NMR spectrometer (Bruker).

\textbf{Figure S1: IR Spectra of (L1a):}

\begin{center}
\includegraphics[width=\textwidth]{ir_spectra}\end{center}

\textbf{IR: 3055(s), 3009(w), 2924(w), 1612(s), 1566(vs), 1466(vs), 1435(vs), 1358(vs), 1304(s), 1242(s), 1149(w), 1095(s), 1041(s), 987(s), 779(vs), 733(s), 663(s), 617(s).}
Figure S2: $^1$H NMR Spectra of L1a:

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.63 (ddd, $J = 4.9, 1.8, 0.9$ Hz, 1H), 8.22 (dt, $J = 8.0, 1.0$ Hz, 1H), 7.74 (ddd, $J = 8.0, 7.5, 1.8$ Hz, 1H), 7.30 (ddd, $J = 7.5, 4.9, 1.2$ Hz, 1H), 2.36 (s, 3H).
Figure S3: $^{13}$C NMR Spectra of L1a:

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 157.42 (s), 155.58 (s), 148.64 (s), 136.20 (s), 124.03 (s), 121.14 (s), 13.87 (s).

\begin{center}
\includegraphics[width=\textwidth]{figure_spectra.png}
\end{center}
Figure S4: Elemental Analysis of L1a

Calculated:

Chemical Formula: C_{14}H_{14}N_{4}
Molecular Weight: 238.29
Elemental Analysis: C, 70.57; H, 5.92; N, 23.51
Figure S5: IR Spectra of L1b:

IR: 3047(w), 3001(w), 2955(w), 1628(vs), 1582(vs), 1466(vs), 1427(vs), 1288(w), 1250(w), 1219(s), 1142(w), 1080(w), 957(s), 864(s), 779(vs), 687(vs), 617(vs), 494(vs)
Figure S6: $^1$H NMR Spectra of L1b:

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.70 (ddd, $J = 4.8, 1.7, 0.9$ Hz, 1H),
8.67 (s, 1H), 8.10 (dt, $J = 7.8, 1.0$ Hz, 1H), 7.78 (td, $J = 7.7, 1.6$ Hz,
1H), 7.34 (ddd, $J = 7.5, 4.8, 1.2$ Hz, 1H).
Figure S7: $^{13}$C NMR Spectra of L1b:

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 162.14 (s), 152.74 (s), 149.94 (s), 136.54 (s), 125.09 (s), 122.49 (s).
Figure S8: Elemental Analysis of L1b:

Calculated:

Chemical Formula: C_{12}H_{10}N_{4}
Molecular Weight: 210.23
Elemental Analysis: C, 68.56; H, 4.79; N, 26.65
Figure S9: IR Spectra of L2a:

IR: 3055(s), 3009(s), 2893(s), 2831(s), 1636(vs), 1558(vs), 1466(vs), 1435(vs), 1358(vs), 1281(vs), 1242(s), 1180(w), 1103(vs), 1041(vs), 987(s), 926(w), 859(w), 787(vs), 656(s), 617(s).
Figure S10: $^1$H NMR Spectra of L2a:

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.58 (ddd, $J$ = 4.8, 1.8, 0.9 Hz, 1H), 8.06 (dt, $J$ = 8.0, 1.0 Hz, 1H), 7.71 - 7.66 (m, 1H), 7.26 (ddd, $J$ = 7.4, 4.8, 1.2 Hz, 1H), 3.96 (s, 2H), 2.42 (s, 3H).
Figure S11: $^{13}\text{C}$ NMR Spectra of L2a:

$^{13}\text{C}$ NMR (101 MHz, CDCl$_3$) $\delta$ 167.50 (s), 157.68 (s), 148.21 (s), 136.26 (s), 124.03 (s), 120.86 (s), 53.49 (s), 14.39 (s).
Figure S12: Elemental Analysis of L2a:

Calculated: 

Chemical Formula: $\text{C}_{16}\text{H}_{18}\text{N}_{4}$

Molecular Weight: 266.34

Elemental Analysis: C, 72.15; H, 6.81; N, 21.04
Figure S13: IR Spectra of L2b:

IR(cm⁻¹ KBr pellet): 3047(s), 3009(w), 2916(s), 2885(vs), 2831(s), 1643(vs), 1566(vs), 1466(vs), 1427(vs), 1335(vs), 1296(s), 1219(s), 1041(vs), 972(vs), 918(vs), 864(vs), 771(vs).
Figure S14: $^1$H NMR Spectra of L2b:

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.60 (ddd, $J$ = 4.8, 1.7, 0.9 Hz, 1H), 8.40 (s, 1H), 7.96 (dt, $J$ = 7.9, 1.0 Hz, 1H), 7.73 – 7.68 (m, 1H), 7.28 (ddd, $J$ = 6.3, 4.2, 1.0 Hz, 1H), 4.04 (s, 2H).
Figure S15: $^{13}$C NMR Spectra of L2b:

$^{13}$C NMR (101 MHz, CDCl$_3$) $\delta$ 163.37 (s), 154.27 (s), 149.33 (s),
136.49 (s), 124.71 (s), 121.29 (s), 61.26 (s).

![13C NMR Spectra of L2b](image)
Figure S16: Elemental Analysis of L2b:

Calibration method: Least Squares to Linear fit
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Calculated:

Chemical Formula: C_{14}H_{14}N_{4}
Molecular Weight: 238.29
Elemental Analysis: C, 70.57; H, 5.92; N, 23.51
Figure S17: IR Spectra of L3a:

IR: 3047(w), 3009(w), 2932(vs), 2878(vs), 1628(vs), 1566(vs), 1466(vs), 1435(vs), 1358(vs), 1304(s), 1227(w), 1103(s), 1072(w), 1041(w), 987(w), 787(vs), 741(s),
Figure S18: $^1$H NMR Spectra of L3a:

$^1$H NMR (400 MHz, CDCl$_3$) δ 8.57 (ddd, $J$ = 4.8, 1.8, 0.9 Hz, 1H), 8.07 (dt, $J$ = 8.0, 1.0 Hz, 1H), 7.68 (ddd, $J$ = 8.0, 7.5, 1.8 Hz, 1H), 7.26 (ddd, $J$ = 7.5, 5.0, 1.2 Hz, 1H), 3.59 (dd, $J$ = 6.3, 5.6 Hz, 2H), 2.36 (s, 3H), 1.93 – 1.89 (m, 2H).
Figure S19: $^{13}$C NMR Spectra of L3a:

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 166.35 (s), 157.83 (s), 148.16 (s), 136.22 (s), 123.93 (s), 120.82 (s), 77.32 (s), 77.00 (s), 76.68 (s), 52.33 (s), 28.93 (s), 13.96 (s).
Figure S20: Elemental Analysis of L3a:

Calculated:

Chemical Formula: $C_{18}H_{22}N_4$
Molecular Weight: 294.39
Elemental Analysis: C, 73.44; H, 7.53; N, 19.03
Figure S21: IR Spectra of L3b:

IR: 3055(s), 3009(s), 2916(vs), 2839(vs), 1636(vs), 1566(vs), 1466(vs), 1435(vs), 1366(s), 1335(vs), 1288(w), 1211(w), 1188(w), 1142(w), 1041(s), 987(vs), 926(s), 895(w), 856(s), 779(vs), 741(s),
Figure S22: $^1$H NMR Spectra of L3b:

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.61 (ddd, $J = 4.8, 1.7, 0.9$ Hz, 1H), 8.36 (s, 1H), 7.95 (dt, $J = 7.9, 1.0$ Hz, 1H), 7.73 - 7.69 (m, 1H), 7.28 (ddd, $J = 7.5, 4.9, 1.2$ Hz, 1H), 3.71 (td, $J = 5.2, 1.4$ Hz, 2H), 1.83 - 1.78 (m, 2H).
Figure S23: $^{13}$C NMR Spectra of L3b:

$^{13}$C NMR (101 MHz, CDCl$_3$) δ 161.88 (s), 154.46 (s), 149.35 (s), 136.47 (s), 124.58 (s), 121.18 (s), 61.18 (s), 28.38 (s).
Figure S24: Elemental Analysis of L3b:

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Calculated:

Chemical Formula: C_{16}H_{18}N_{4}
Molecular Weight: 266.34
Elemental Analysis: C, 72.15; H, 6.81; N, 21.04
Figure S25: ORTEP of L1a
Figure S26: ORTEP of L2a

Figure S27: ORTEP of L3b:
Figure S28: Solid State UV-Vis Spectrum of L1a:

![UV-Vis Spectrum of L1a](image)

Figure S29: Solid State UV-Vis Spectrum of L2a:

![UV-Vis Spectrum of L2a](image)
Figure S30: Solid State UV-Vis Spectrum of L3b:
Figure S31: Excitation Spectra of L1b in CHCl$_3$ in different concentrations: (a) $10^{-3}$M, (b) $10^{-4}$M, (c) $10^{-5}$M
Figure S32: PL Spectra of L1b in CHCl3 in different Concentrations: (a) $10^{-4}$M; (b) $10^{-5}$M
Figure S33: Excitation Spectra of L2a in CHCl₃ in different concentrations: (a) $5 \times 10^{-2}$M (b) $10^{-2}$M (c) $5 \times 10^{-3}$M, (d) $10^{-3}$M (Emission Wavelength is kept at 370 nm)
Figure S34: Excitation Spectra of L3a in CHCl₃ in different concentrations: (a) 5×10⁻¹M (b) 2×10⁻¹M; (c) 10⁻¹M (d) 5×10⁻²M, (e) 10⁻²M, (f) 5×10⁻³M; (g) 10⁻³M (Emission Wavelength is kept at 460 nm)
Figure S35: PL Spectra of L3a in CHCl₃ in different concentrations: (a) \(5 \times 10^{-1}\) M (b) \(2 \times 10^{-1}\) M; (c) \(10^{-1}\) M (d) \(5 \times 10^{-2}\) M, (e) \(10^{-2}\) M, (f) \(5 \times 10^{-3}\) M; (g) \(10^{-3}\) M. (Excitation Wavelength is kept at 420 nm)
Figure S36: PL Spectra (at an excitation wavelength of 450 nm) of L3a in solid state

![PL Spectra Diagram](image-url)
Figure S37: $^1$H NMR spectra of L3b in CDCl$_3$ by changing the concentration of compound; (a) 1 M; (b) $10^{-1}$ M; (c) $10^{-2}$ M; (d) $10^{-3}$ M
Figure S38: NOESY of L3b in CDCl₃ at a concentration of 1 M
Figure S39: NOESY of L3b in CDCl$_3$ at a concentration of $10^{-2}$ M
**Compound L1a**

checkCIF/PLATON (full publication check)

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

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Click on the hyperlinks for more details of the test.

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More ...

Alert level C

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And 4 other PLAT230 Alerts
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And 2 other PLAT241 Alerts
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PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.10 Report
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PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ........ 18 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
4 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected
**Compound L2a**

checkCIF/PLATON (full publication check)

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Click on the hyperlinks for more details of the test.

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- PLAT147_ALERT_1_C su on Symmetry Constrained Cell Angle(s) ...... Please Check
- PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C6A Check
- PLAT340_ALERT_3_C Low Bond Precision on  C-C Bonds ............... 0.0048 Ang.
- PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
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**Alert level G**
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- PLAT153_ALERT_1_G The su's on the Cell Axes are Equal ........ 0.00500 Ang.
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- PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note

0 ** ALERT level A** = Most likely a serious problem - resolve or explain
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**Compound L3b**

**checkCIF/PLATON (full publication check)**

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<td>0.074</td>
<td>0.074</td>
</tr>
<tr>
<td>F000</td>
<td>284.0</td>
<td>284.0</td>
</tr>
<tr>
<td>F000'</td>
<td>284.08</td>
<td></td>
</tr>
<tr>
<td>h,k,lmax</td>
<td>11,11,11</td>
<td>11,11,11</td>
</tr>
<tr>
<td>Nref</td>
<td>1451</td>
<td>1448</td>
</tr>
</tbody>
</table>
Tmin, Tmax  0.982, 0.985  0.926, 1.000
Tmin'  0.978

Correction method= # Reported T Limits: Tmin=0.926 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998  Theta(max)= 26.000
R(reflections)= 0.0445 (993)  wR2(reflections)= 0.1214 (1448)
S = 1.042  Npar= 91

The following ALERTS were generated. Each ALERT has the format

  test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

**Alert level G**

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF  Please Do!

PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)  293 Check

PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K)  293 Check

PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL  2014 Note

0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
4 ALERT level G = General information/check it is not something unexpected