Supporting Information

Experimental Study on Arsoles; Structural Variation, Optical and Electronic Properties, and Emission Behavior

Makoto Ishidoshiro, Hiroaki Imoto, Susumu Tanaka, Kensuke Naka*

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### 2. Crystallographic data

#### Table S1. Crystallographic Data.

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<th>5d</th>
<th>5e</th>
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<td>C\textsubscript{22}H\textsubscript{15}AsBr\textsubscript{2}</td>
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<td>Formula weight</td>
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<td>514.09</td>
<td>442.43</td>
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<td>monoclinic</td>
<td>monoclinic</td>
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<td>Space group</td>
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<td>P\textsubscript{2}\textsubscript{1}</td>
<td>P2\textsubscript{1}/n</td>
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<td>-</td>
<td>-</td>
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<td>β [°]</td>
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<td>98.216(7)</td>
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#### Data Collection

| Temperature [°C] | 23.0 | 23.0 | 23.0 |
| 2θ\textsubscript{max} [°] | 55.1 | 55.0 | 55.1 |
| Tmin/Tmax | 0.605 / 0.788 | 0.624 / 0.708 | 0.833 / 0.953 |

#### Refinement

| No. of Observed Data | 8824 | 4562 | 4948 |
| No. of Parameters | 451 | 244 | 262 |
| R1\textsuperscript{a}, wR2\textsuperscript{b} | 0.0620, 0.0890 | 0.0440, 0.1158 | 0.0541, 0.1224 |

\[ \text{R1} = \Sigma | |Fo| - |Fc| / \Sigma |Fo| \]
\[ \text{wR2} = [ \Sigma w ((Fo^2-Fc^2)^2 / \Sigma w (Fo^2)^2)]^{1/2} \]
\[ w = \left[ \sigma(Fo^2) \right]^{-1} \]

CCDC #1449110 (5b), 1449111 (5d), and 1449112 (5e).

The crystallographic data of 5a, 5c, and 6a have been reported in the previous literature.\textsuperscript{[1]}
Table S2. ORTEP drawing (ellipsoids at 50% probability), selected angles (deg) and distance (Å) of 5b.

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| Angle (°)              | C(1)-As(1)-C(4) | 87.3(4) |

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*S10*
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Table S3. ORTEP drawing (ellipsoids at 50% probability), selected angles (deg) and distance (Å) of 5d.

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### Table S4. ORTEP drawing (ellipsoids at 50% probability), selected angles (deg) and distance (Å) of 5e.

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Figure S14 (a) Packing structure of 5a. The hydrogen atoms are omitted for clarity. (b) Intermolecular CH-π interaction.

Figure S15 (a) Packing structure of 5b. The hydrogen atoms are omitted for clarity. (b) Intermolecular CH-π interaction.
Figure S16 (a) Packing structure of 5c. The hydrogen atoms are omitted for clarity. (b) Intermolecular CH-π interaction.

Figure S17 (a) Packing structure of 5d. The hydrogen atoms are omitted for clarity. (b) Intermolecular CH-π interaction.
3. Optical properties

**Figure S18.** PL spectra of $5_{\text{cry}}$ and $5_{\text{grd}}$ (excited at 350 nm).

**Figure S19.** PL spectra of $5e$ in various solvents.
4. CV data

**Figure S20.** Cyclic voltammograms of (a) 5a, (b) 5b, (c) 5c, (d) 5d, (e) 5e and (f) 6a measured in THF solutions \((c = 0.1 \text{ M})\) at the scan rate of 100 mV/s under N\(_2\). The working electrode was a glassy carbon, the counter electrode was a platinum wire, and the reference electrode was an Ag\(^0\) / Ag\(^+\).

**Figure S21.** Cyclic voltammograms of 5a measured in THF solutions \((c = 0.1 \text{ M})\) at the scan rate of 100 mV/s under N\(_2\). The working electrode was a glassy carbon, the counter electrode was a platinum wire, and the reference electrode was an Ag\(^0\) / Ag\(^+\).
5. XRD patterns

Figure S22. XRD patterns of $5e_{\text{solv}}$ and $5e_{\text{grd}}$, and simulated PXRD of $5e_{\text{cry}}$. 
6. Theoretical calculations

Figure S23. Molecular orbitals of the HOMO and LUMO. The geometries were optimized by DFT calculation at the B3LYP/6-31G+(d) level of theory; calculated with the Gaussian 09 suit program.[2]
Table S5. Calculated energy levels, HOMO-LUMO transition energies, and torsion angles.\textsuperscript{a}

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<th>Single crystal XRD\textsuperscript{c}</th>
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\textsuperscript{a}All calculation were performed at the B3LYP/6-31G+(d) level of theory with the Gaussian 09 suit program. \textsuperscript{b}Structures optimized by DFT calculation. \textsuperscript{c}Structures obtained by single crystal X-ray diffraction. \textsuperscript{d}DFT calculation. \textsuperscript{e}TD-DFT calculation. \textsuperscript{f}Torsion angles of the cyclopentadiene and aryl groups. \textsuperscript{g}5b adopt two different conformations in the single crystal.
**Table S6.** Atom coordinates and absolute energy levels for 5a optimized in the S0 state.

5a (S0 state): E(RB3LYP) = -3082.40024809 A.U.

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Table S7. Atom coordinates and absolute energy levels for 5b optimized in the $S_0$ state.

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S23
Table S9. Atom coordinates and absolute energy levels for 5d optimized in the S₀ state.

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**S24**
Table S10. Atom coordinates and absolute energy levels for 5e optimized in the S_0 state.

5e (S_0 state): E(RB3LYP) = -3350.34343066 A.U.

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Table S11. Atom coordinates and absolute energy levels for 6a optimized in the $S_0$ state.

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