Electronic Supplementary Information

Exploring the Coordination Chemistry of Bifunctional Organoarsenate Ligands: Syntheses and Characterisation of Coordination Polymers that Contain 4-(1, 2, 4-triazol-4-yl)phenylarsonic Acid

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c Univ. Bordeaux, CRPP, UPR 8641, F-33600 Pessac, France.
d School of Physics & CRANN, University of Dublin, Trinity College, Dublin 2, Ireland.

Table S1.1 Selected bond lengths (Å) and angles (°) of 1.

<table>
<thead>
<tr>
<th>Bond</th>
<th>Length (Å)</th>
<th>Bond</th>
<th>Length (Å)</th>
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<td>As1B—O11</td>
<td>1.572 (3)</td>
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<tr>
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<td>As1A—O12</td>
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Symmetry codes: (i) x, y−1, z; (ii) x+1, y, z; (iii) x−1, y, z; (iv) x, y+1, z.

Table S1.2 Hydrogen-bond geometry (Å, °) of 1.

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<td>1.92</td>
<td>2.659 (3)</td>
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Symmetry codes: (i) x, y−1, z; (iv) x, y+1, z; (v) −x+3/2, y−1/2, −z+1/2.

Table S2.1 Selected bond lengths (Å) and angles (°) of 2.

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Symmetry codes: (i) x, −y, z; (ii) −x+3/2, −y+1/2, −z+1; (iii) −x+1, y, −z+1; (iv) x+1/2, −y+1/2, z.

**Table S2.2** Hydrogen-bond geometry (Å, °) of 2.

<table>
<thead>
<tr>
<th>D—H···A</th>
<th>D—H</th>
<th>H···A</th>
<th>D···A</th>
<th>D—H···A</th>
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**Table S3.1** Selected bond lengths (Å) and angles (°) of 3.

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<td>O1—Co1—N1&quot;</td>
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<td>N1&quot;—Co1—Cl1&quot;</td>
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Symmetry codes: (i) x, −y, z; (ii) −x+1/2, −y+1/2, −z; (iii) x−1/2, y+1/2, z; (iv) −x+1, −y, −z.

**Table S3.2** Hydrogen-bond geometry (Å, °) of 3.

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<tr>
<th>D—H···A</th>
<th>D—H</th>
<th>H···A</th>
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**Table S4.1** Selected bond lengths (Å) and angles (°) of 4.

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3
<table>
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<th>Bond</th>
<th>Length (Å)</th>
<th>Angle (°)</th>
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<td>N21—Mn1—N11</td>
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<td>O11&quot;—Mn1—N21</td>
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Symmetry codes: (i) −x+1, y+1/2, −z+3/2; (ii) x, −y+1/2, z+1/2; (iii) −x, y−1/2, −z+5/2; (iv) x, −y+3/2, z−1/2; (v) −x+1, y−1/2, −z+3/2; (vi) x, −y+1/2, z−1/2; (vii) −x, y+1/2, −z+5/2; (viii) x, −y+3/2, z+1/2.

**Table S4.2** Hydrogen-bond geometry (Å, °) of 4.

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<th>D—H···A</th>
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Symmetry codes: (ix) −x+1, −y+1, −z+2; (x) −x, −y+1, −z+2.

**Table S5.1** Selected bond lengths (Å) and angles (°) of 5.

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Symmetry codes: (i) −x+1, y−1/2, −z+1/2; (ii) x, −y+3/2, z+1/2; (iii) −x, y+1/2, −z+3/2; (iv) x, −y+1/2, z−1/2; (v) −x+1, y+1/2, −z+1/2; (vi) x, −y+3/2, z−1/2; (vii) −x, y−1/2, −z+3/2; (viii) x, −y+1/2, z+1/2.

Table S5.2 Hydrogen-bond geometry (Å, °) of 5.

<table>
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<th>H···A</th>
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<td>O13—H13···O22(x)</td>
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<td>1.67</td>
<td>2.510 (2)</td>
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<td>O23—H23···O12(x)</td>
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<td>1.69</td>
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Symmetry codes: (ix) −x+1, −y+1, −z+1; (x) −x, −y+1, −z+1.
Fig. S1 (a) The asymmetric unit of 1. (b) Intramolecular and intermolecular hydrogen bonds in 1. The blue dashed lines (2.659 and 2.771 Å) stand for intramolecular hydrogen bonds, the orange dashed lines (2.473 Å) stand for intermolecular hydrogen bonds.
Fig. S2 (a) The asymmetric unit of 2. (b) Polyhedral representation of intramolecular and intermolecular hydrogen bonds in 2. The blue dashed lines (2.661 Å) stand for intramolecular hydrogen bonds, the orange dashed lines (2.839 and 2.845 Å) stand for intermolecular hydrogen bonds.
Fig. S3 (a) The asymmetric unit of 3. (b) The coordination environment of Co(II) ion and the coordination modes of the ligands in 3. Symmetry codes: (i) $x, -y, z$; (ii) $-x+1/2, -y+1/2, -z$; (iii) $x-1/2, y+1/2, z$; (iv) $-x+1, -y, -z$; (v) $-x+1/2, y-1/2, -z$; (vi) $x+1/2, y-1/2, z$; (vii) $-x+1/2, y+1/2, -z$; (viii) $-x+1, y, -z$. (c) Polyhedral representation of the 1-D substructure along the $b$-axis in 3 involving Co(II) and Cl$^-$ and the As$1$O$_3$ moiety. (d) Polyhedral representation of the two-dimensional layer structure of 3. (e) Polyhedral representation of intramolecular and intermolecular hydrogen bonds in 3. The blue dashed
lines (2.644 and 2.774 Å) stand for intramolecular hydrogen bonds, the orange dashed lines (2.793 Å) stand for intermolecular hydrogen bonds.

Fig. S4 (a) The asymmetric unit of 4. (b) Polyhedral representation of the topological simplification fashion in 4.
(a)

(b)

(c)
Fig. S5 The power X-ray diffraction patterns for compounds 1–5.
(a) Compound 1

(b) Compound 2
(c) Compound 3

(d) Compound 4
(e) Compound 5

(f) H$_2$TPAA

Fig. S6 IR spectra of compounds 1–5 (a-e) and H$_2$TPAA (f).
Fig. S7 Photoluminescent spectra of ligand H₂TPAA in the solid state at room temperature.

Fig. S8 TGA curves for compounds 1–5.
Fig. S9 $^1$H NMR of H$_2$TPAA in DMSO-d$_6$. The strong peak at 3.7205 ppm should be $^1$H peak of water which could be caused by the recrystallization of H$_2$TPAA from water. 2.5088 ppm is the $^1$H peak of DMSO-d$_6$. 
Fig. S10 $^{13}$C NMR of H$_2$TPAA in DMSO-d$_6$. The strong peak at 39.4123 ppm is the $^{13}$C NMR peak of DMSO-d$_6$.

Fig. S11 The structure of H$_2$TPAA.
Fig. S12 Field dependence of reduced magnetization at the temperatures indicated for 3.

Fig. S13 Temperature dependence below 15 K of the in- and out-of-phase components of ac susceptibility for 3 at 1000 Hz with an amplitude of the ac field of 3 Oe.