The importance of Au…π(aryl) interactions in the formation of spherical aggregates in binuclear phosphanegold(I) complexes of a bipodal thiocarbamate dianion: A combined crystallographic and computational study, and anti-microbial activity†

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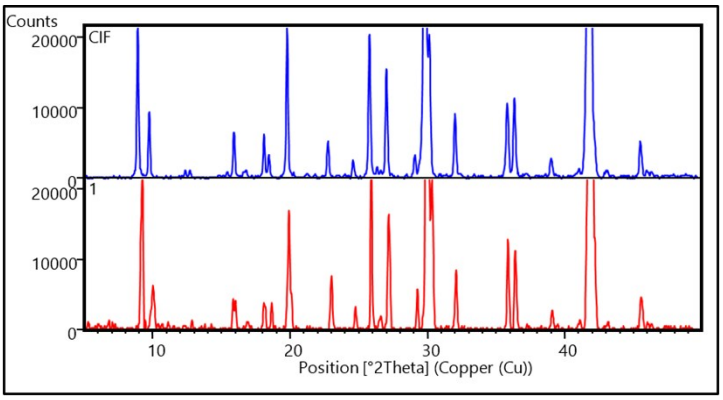
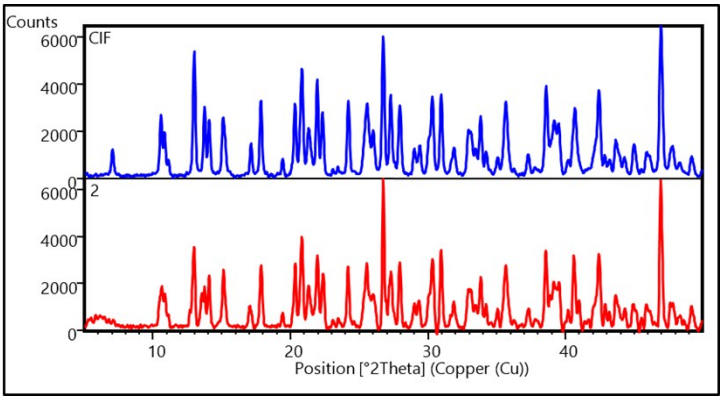
ELECTRONIC SUPPLEMENTARY INFORMATION

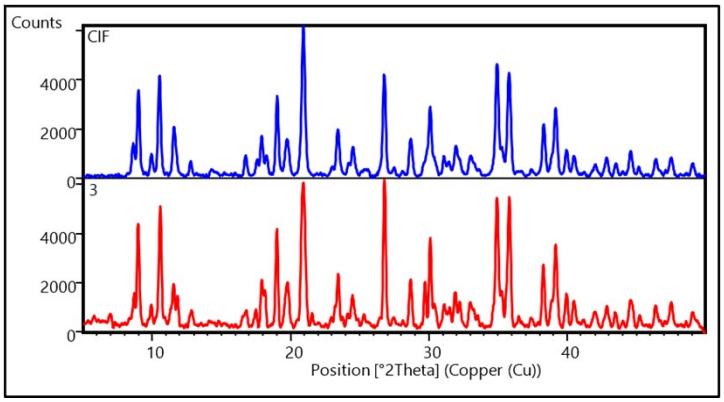
Figure S(1). Experimental (red trace) and simulated based on the single crystal structure (blue trace) PXRD patterns for (a) **1**, (b) **2** and (c) **3**. These show that the single crystal data reported herein for each of **1**–**3** match the structure of the bulk material in each case.



(a)

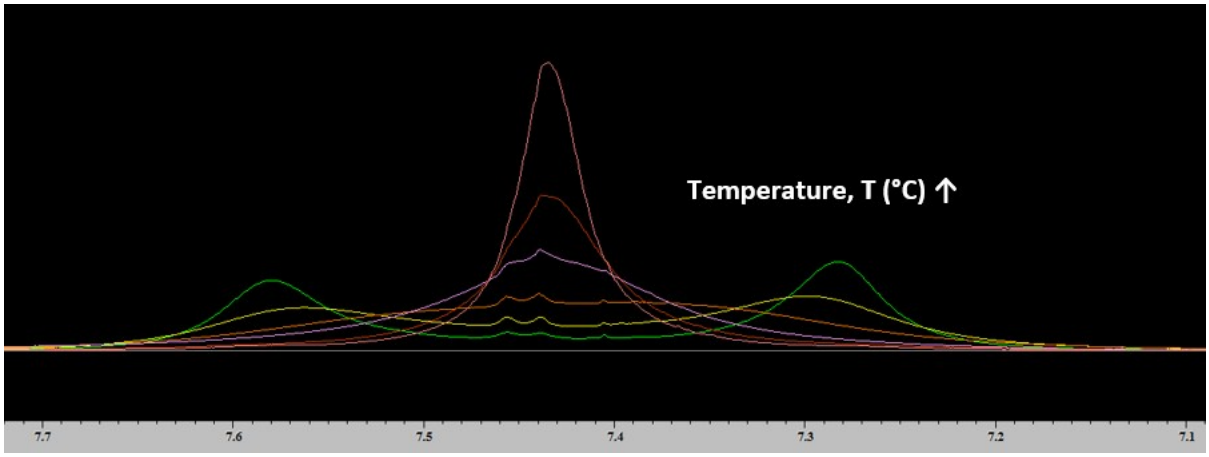


(b)

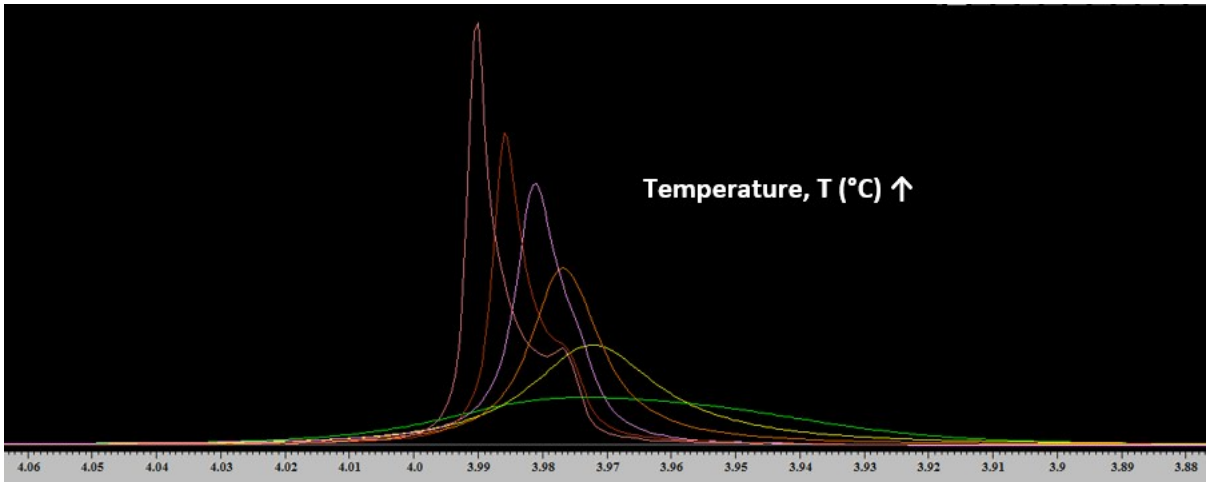


(c)

Figure S(2). Variable ^{1}H NMR study in DMSO-d6 for LH_2: (a) coalescence in the resonances due to aryl-H with increasing temperature, and (b) sharpening and downfield shift in the resonances due to methyl-H with increasing temperature. The temperature range was 28–78 °C with 10 °C increments.

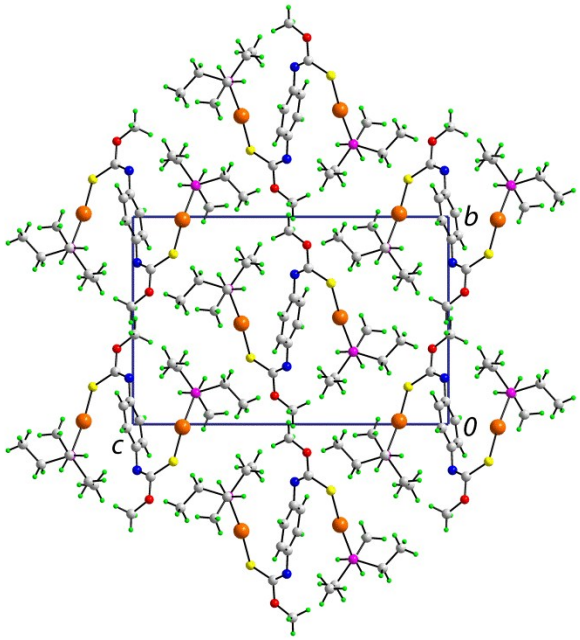


(a)

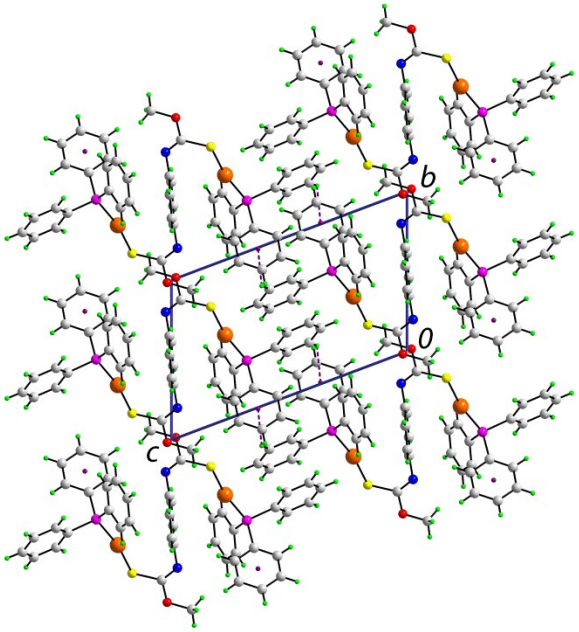


(b)

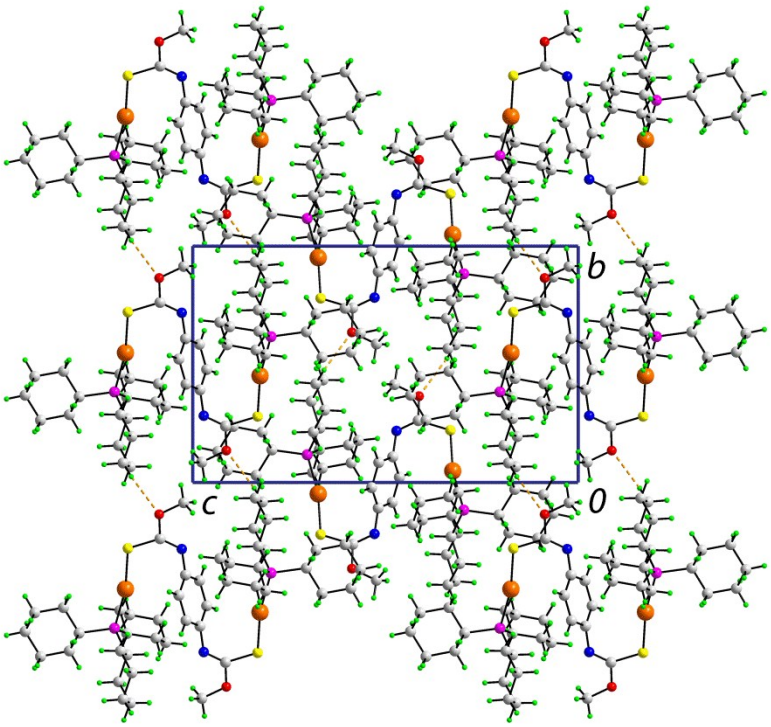
Figure S(3). Crystal packing diagrams for (a) **1**, (b) **2** and (c) **3**, viewed in projection down the *a*-axis in each case. In **2**, there are phenyl-C–H…π(aryl) interactions [C23–H23…Cg(C31-C36) = 2.82 Å, C23…Cg(C31-C36) = 3.599(4) Å with angle at H23 = 140° for symmetry operation: 2-*x*, 2-*y*, 1-*z*] shown as purple dashed lines, and in **3**, there are methylene-C–H…O interactions shown as orange dashed lines [C14–H14a…O1 = 2.58 Å, C14…O1 = 3.266(3) Å with angle at H14a = 127° for symmetry operation: *x*, -1+*y*, *z*].



(a)

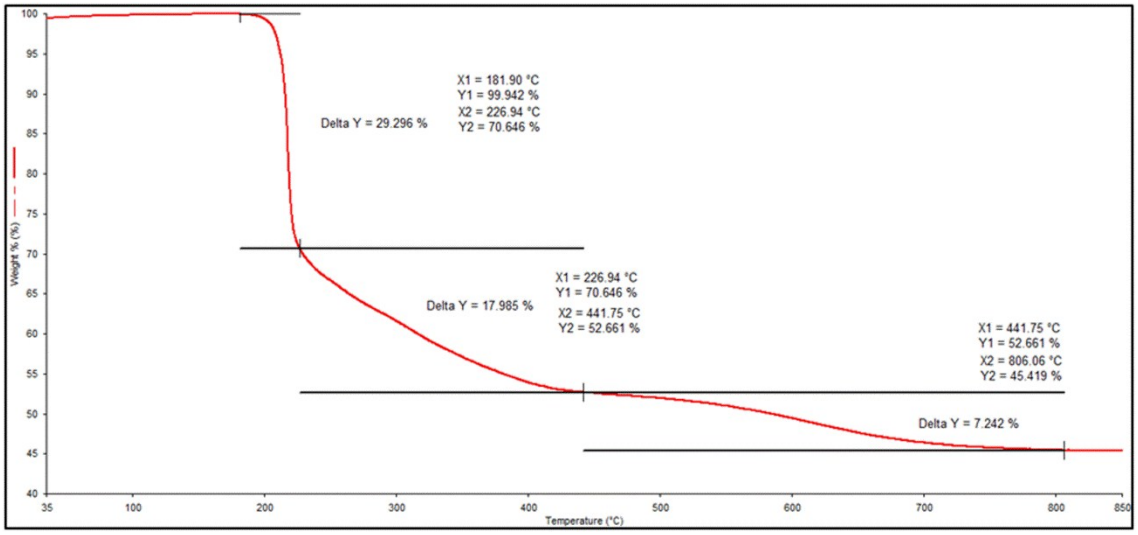


(b)

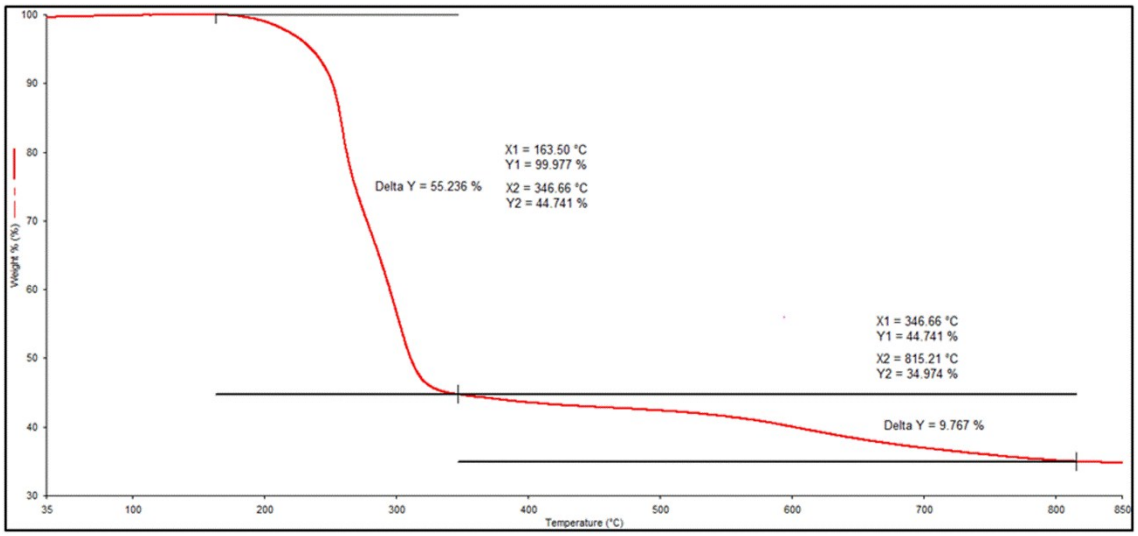


(c)

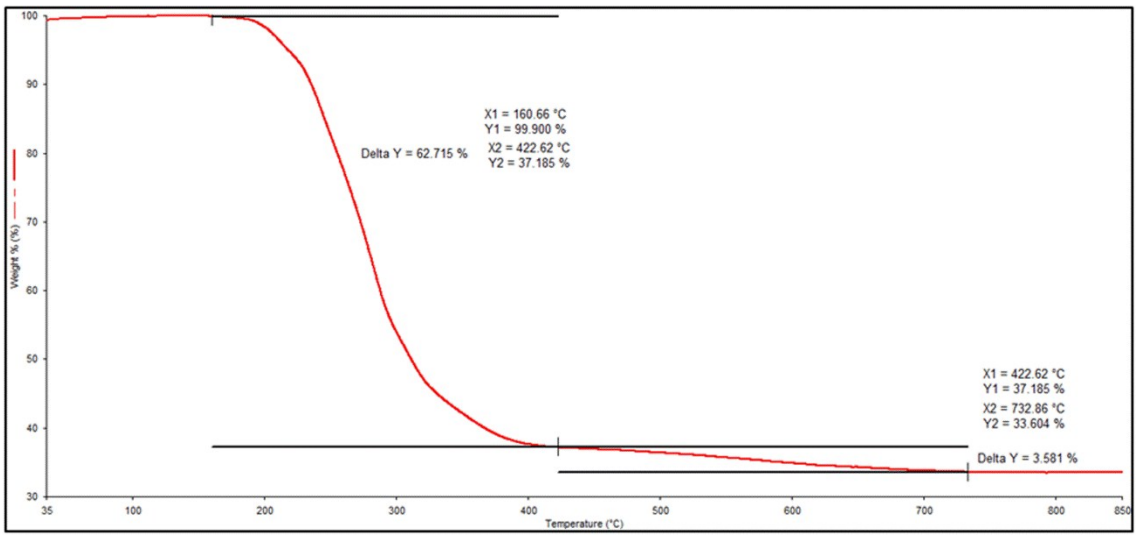
Figure S(4). Thermogravimetric traces for (a) **1**, (b) **2** and (c) **3**.



(a)



(b)


X1 = 160.66 °C
Y1 = 99.900 %
Delta Y = 62.715 %
X2 = 422.62 °C
Y2 = 37.185 %
X1 = 422.62 °C
Y1 = 37.185 %
X2 = 732.86 °C
Y2 = 33.604 %
Delta Y = 3.581 %
Weight % (%)
Temperature (°C)

(c)