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 ###

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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.
Figure S(2). Variable $^1$H NMR study in DMSO-d$_6$ 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.
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].
Figure S(4). Thermogravimetric traces for (a) 1, (b) 2 and (c) 3.