Easy imine formation assisted by heteropolynuclear gold-thallium complexes

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Supplementary Material

Table S1. Details of data collection and structure refinement for complex **1a.**

Compound	**1a**
Chemical formula	$C_{14}H_8AuCl_{10}N_2Tl$
Crystal color	colorless
Crystal size / mm	0.30 x 0.30 x 0.05
Crystal system	Monoclinic
Space group	$P2_1/c$
a / Å	20.5626(5)
b / Å	6.8262(2)
c / Å	17.2914(9)
α / º	90
β / º	111.8915(14)
γ / º	90
Volume / Å^3	2252.08(15)
Z	4
D_c / g·cm^{-3}	2.832
F(000)	1744
Temperature	173(2) K
$2\theta_{max}$ / º	47.10
μ (Mo-$K\alpha$) /mm^{-1}	14.846
No. of reflections measured	11238
No. of unique reflections	3291
R_{int}	0.1321
R [a] (I>2σ(I))	0.0697
wR [b] (F^2, all refl.)	0.1960
No. of parameters	262
No. of restraints	69
S [c]	1.141
Max. residual electron density / e·Å^{-3}	3.175

[a] $R(F) = \Sigma\, ||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR(F^2) = [\Sigma\{w(F_o^2-F_c^2)^2\}/\ \Sigma\{w(F_o^2)^2\}]^{0.5}$; $w^{-1} = \sigma^2(F_o^2)+(aP)^2+bP$, where $P = [F_o^2+2F_c^2]/3$ and a and b are constants adjusted by the program. [c] $S = [\Sigma\{w(F_o^2-F_c^2)^2\}/(n-p)]^{0.5}$, where n is the number of data and p the number of parameters.

Table S2. Selected bond lengths [Å] and angles [°] for complex **1a**.

Au-C(11)	2.007(17)	Tl-N(1)	2.650(18)
Au-C(1)	2.074(17)	Tl-N(2)	2.654(16)
Au-Tl	3.0992(18)		
C(11)-Au-C(1)	179.2(4)	N(1)-Tl-N(2)	68.7(5)
C(11)-Au-Tl	88.8(3)	N(1)-Tl-Au	81.3(3)
C(1)-Au-Tl	91.9(3)	N(2)-Tl-Au	86.7(3)

Figure S1. Molecular structure of complex **1a** with the labeling scheme of the atom positions.

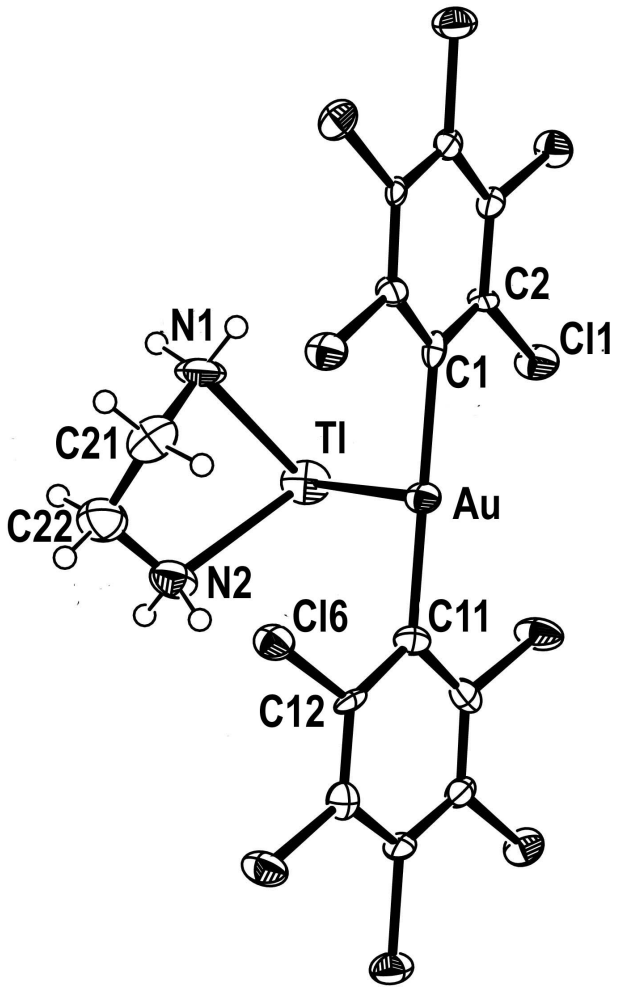
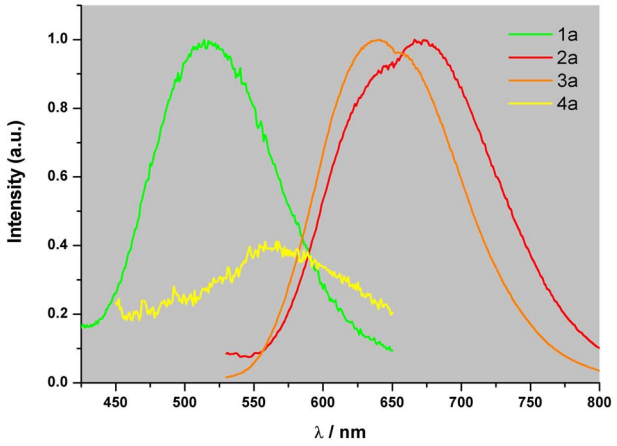


Figure S2. Normalized emission spectra in solid state of the complexes **1a**-**4a** and **1b**-**4b**.



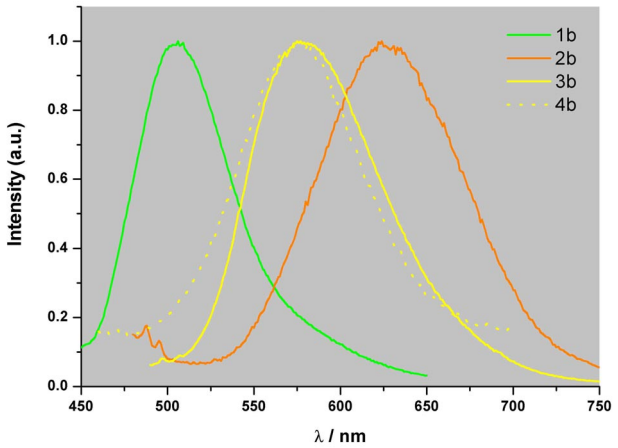


Figure S3. Crystal structure of complex **2a** viewed perpendicular to the polymetallic chain.

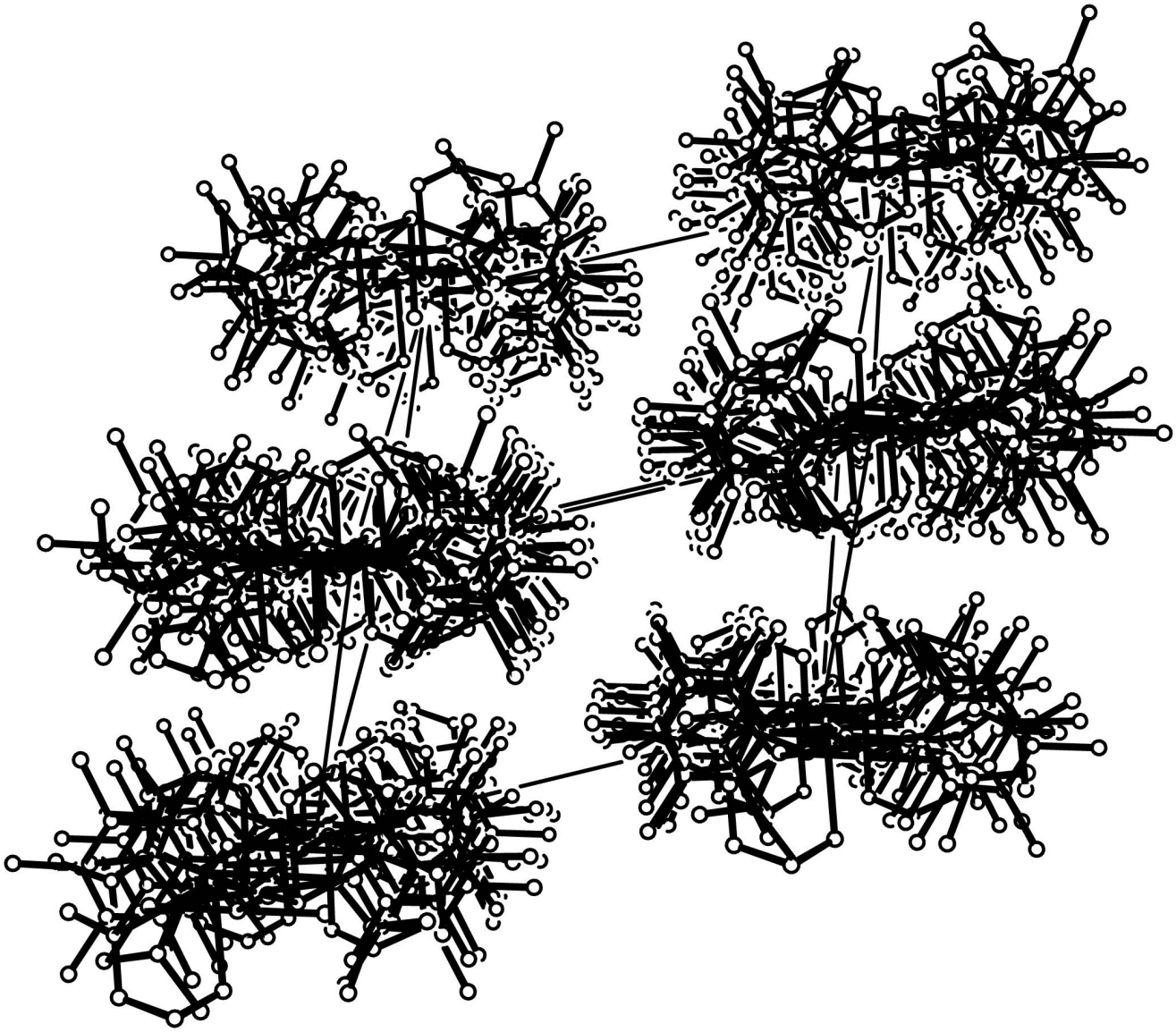


Figure S4. Crystal structure of complex **2a** viewed parallel to the polymetallic chain.

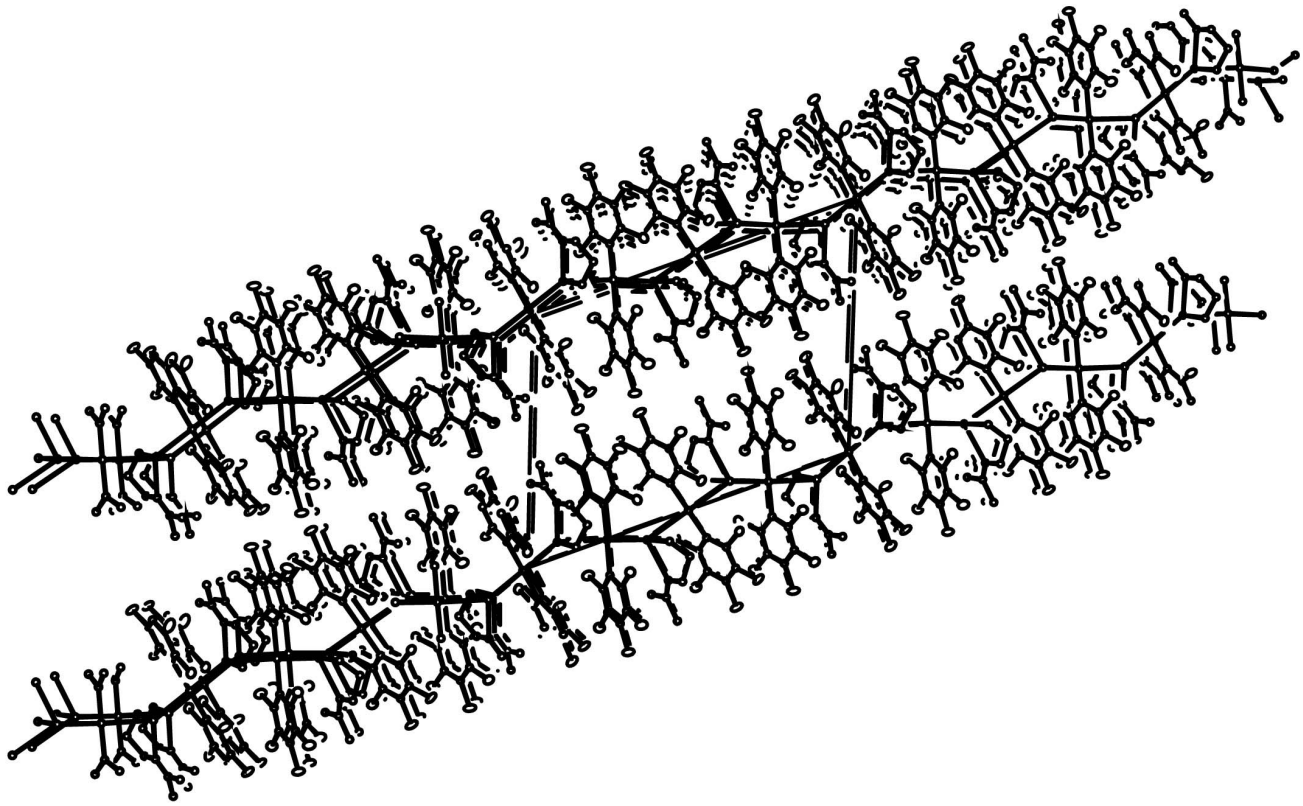


Figure S5. Crystal structure of complex **3a** viewed perpendicular to the polymetallic chain.

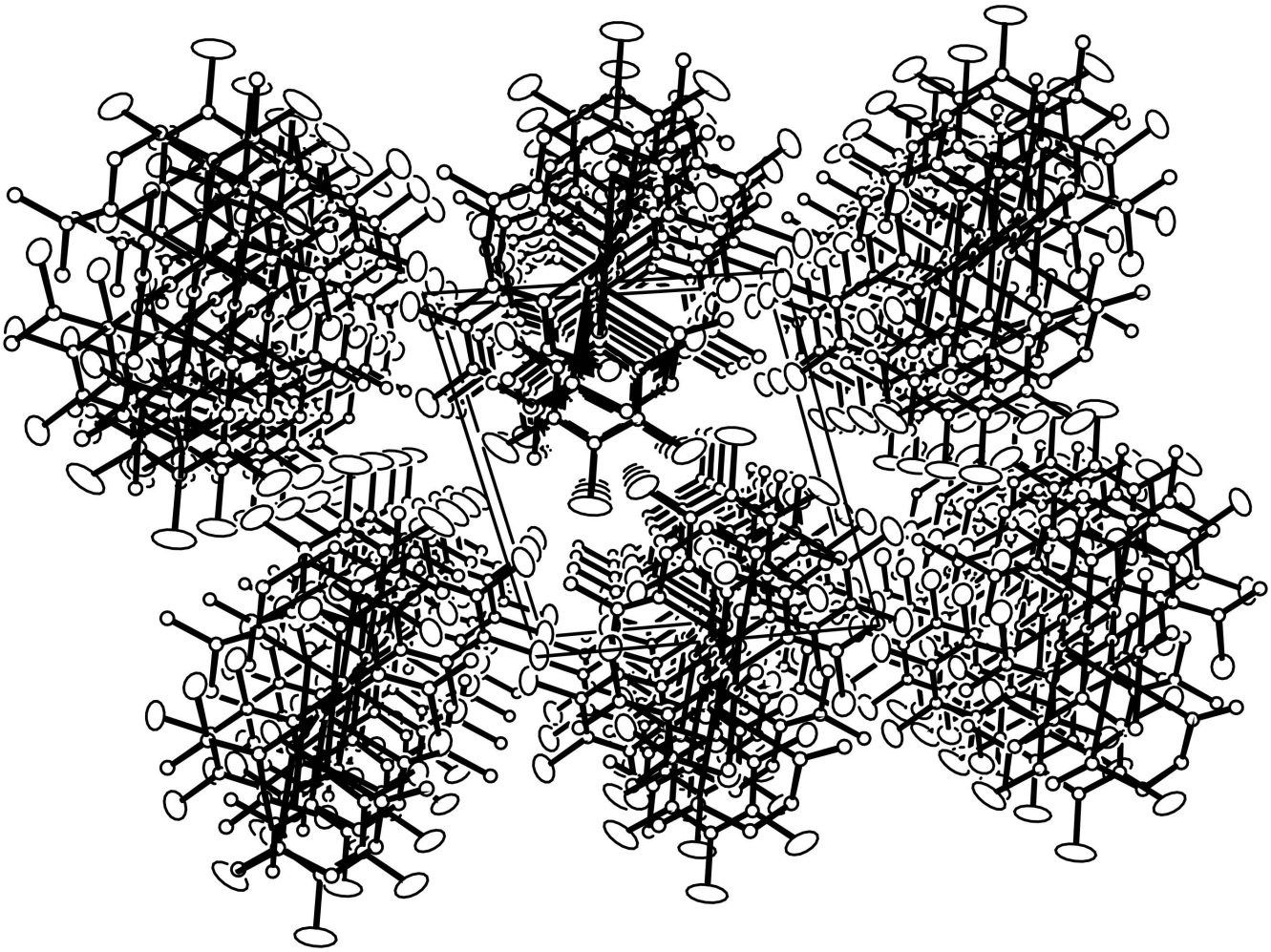


Figure S6. Crystal structure of complex **3a** viewed parallel to the polymetallic chain.

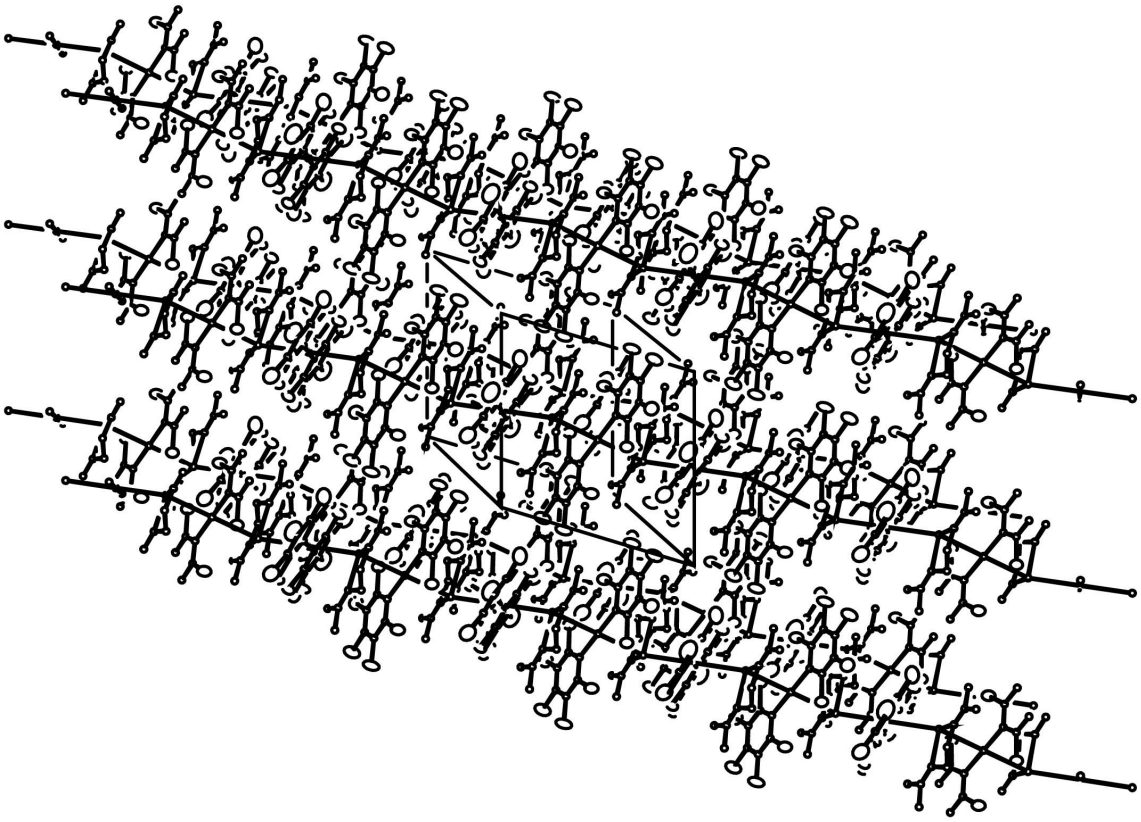


Figure S7. Crystal structure of complex **3b** viewed perpendicular to the polymetallic chain.

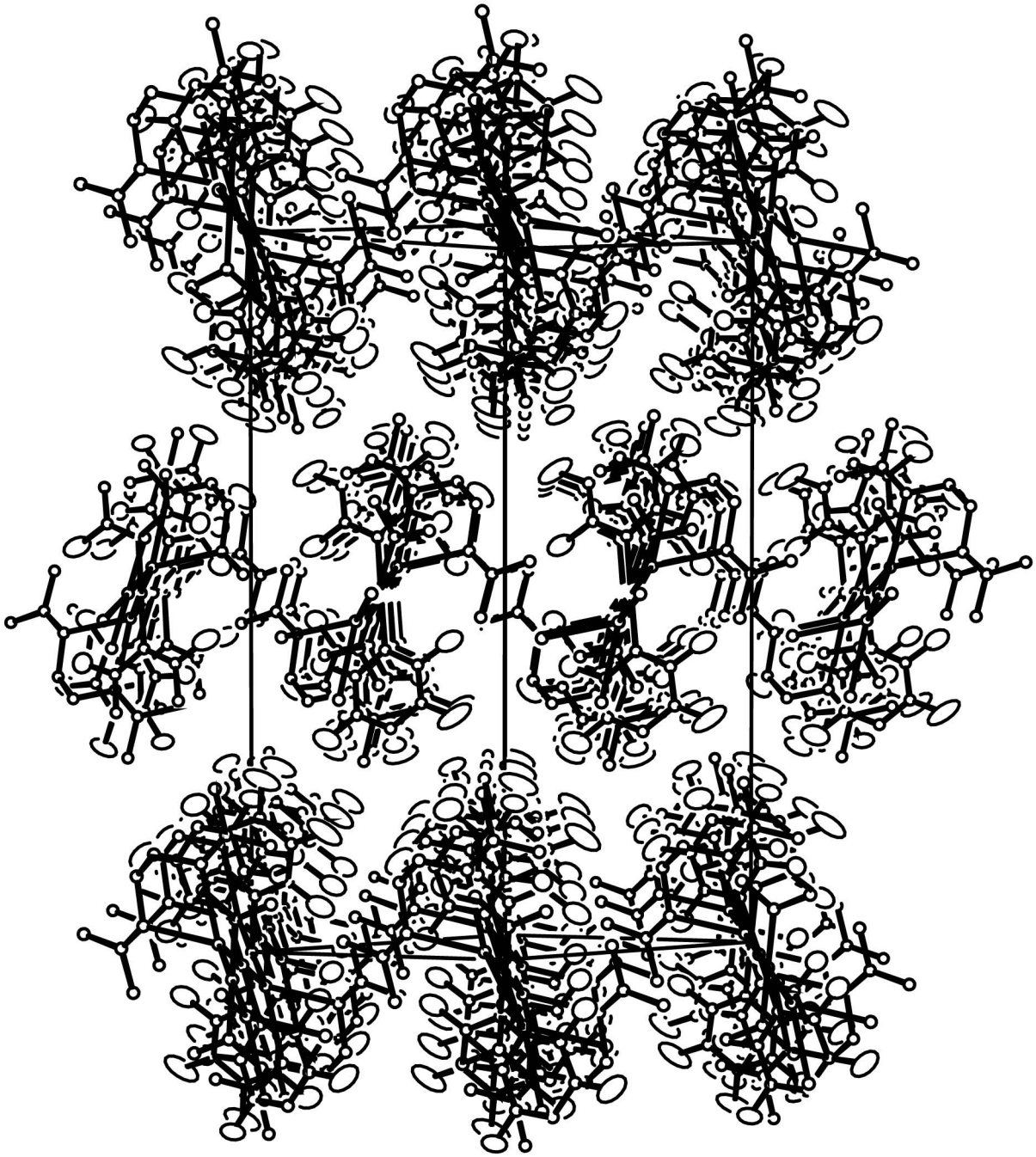
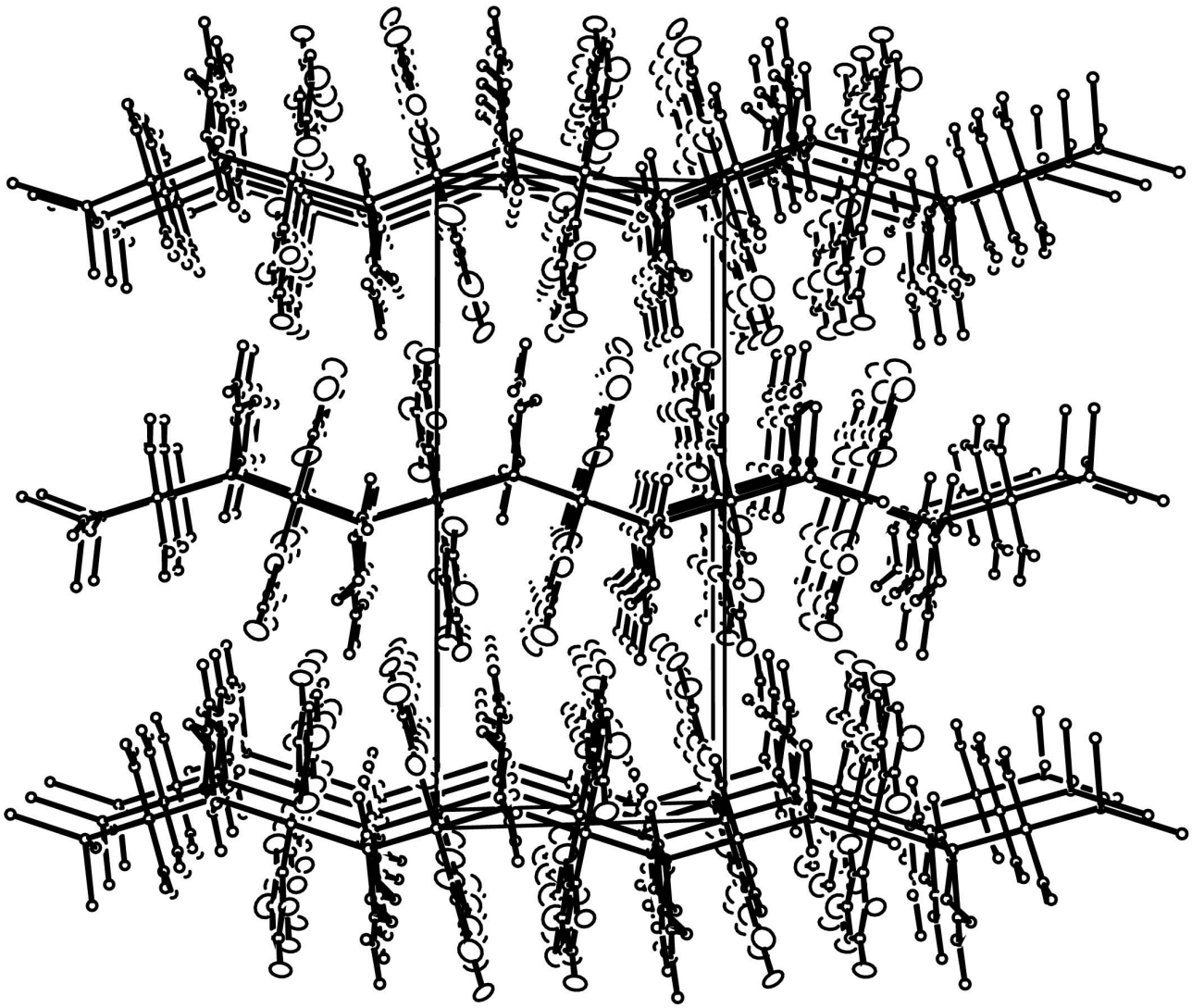



Figure S8. Crystal structure of complex **3b** viewed parallel to the polymetallic chain.