

Supporting Information

A Dynamic Tetranuclear Gold(I)-Cyclophane – Gold(I)-Centred Chirality and Fluxionality Arising from Intramolecular Shift of Au-S Bonds

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Table S1 Crystal data of 1·2Et₂O	
Compounds	1·2Et₂O
Empirical formula	C ₉₆ H ₈₄ Au ₄ O ₂ P ₄ S ₄
Formula weight	2309.61
Crystal system	triclinic
Space group	<i>P</i> $\bar{1}$
Unit cell dimensions	
<i>a</i> (Å)	12.8550(6)
<i>b</i> (Å)	13.0540(7)
<i>c</i> (Å)	13.8019(7)
α (°)	109.2250(16)
β (°)	99.6320(17)
γ (°)	100.9310(16)
Volume (Å ³)	2080.26(18)
<i>Z</i>	1
Calculated density (g cm ⁻³)	1.844
Absorption coefficient (mm ⁻¹)	7.258
<i>F</i> (000)	1116
Crystal size (mm ³)	0.060 × 0.070 × 0.200
θ range for data collection (°)	2.05 to 28.34
Index ranges	-17 ≤ <i>h</i> ≤ 17, -14 ≤ <i>k</i> ≤ 17, -18 ≤ <i>l</i> ≤ 18
Reflections collected	45591
Independent reflections [<i>R</i> (int)]	10343 0.0401
Max. and min. transmission	0.7457 and 0.5648
Data/restraints/parameters	10343 / 0 / 498
Goodness-of-fit	1.036
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0272, <i>wR</i> 2 = 0.0596
Largest diff. peak and hole (e.Å ⁻³)	2.582 and - 1.412

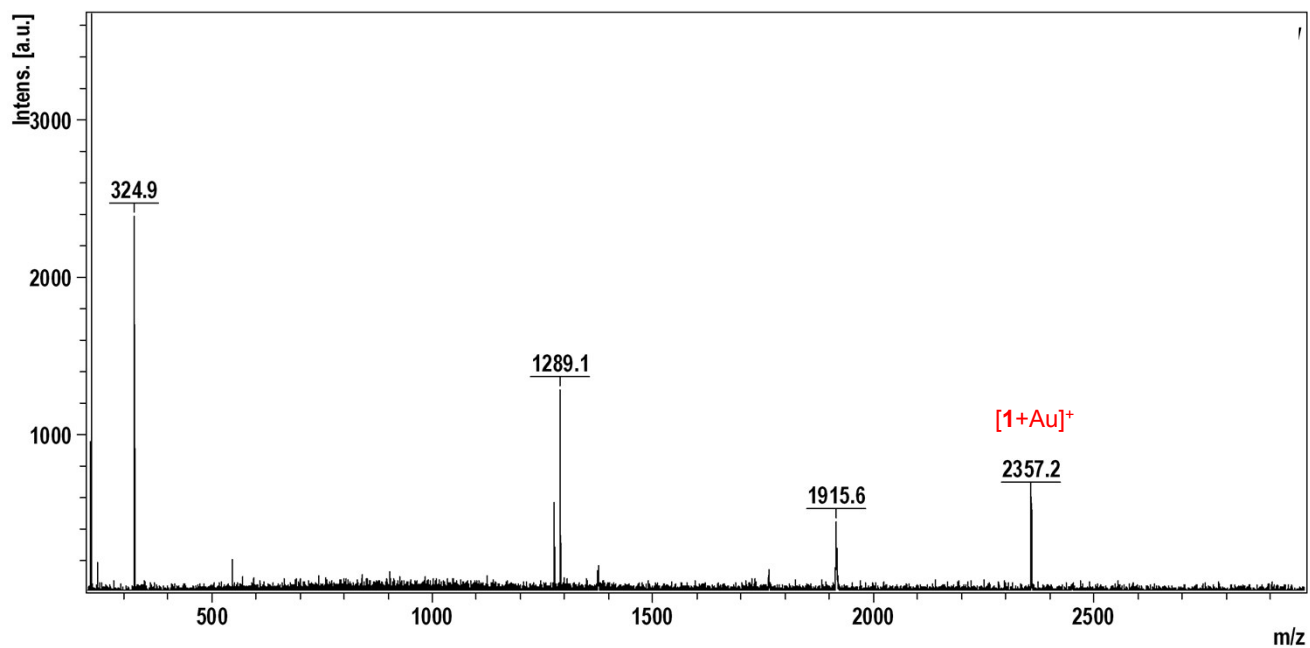


Figure S1 MALDI-TOF mass spectrum of **1**.

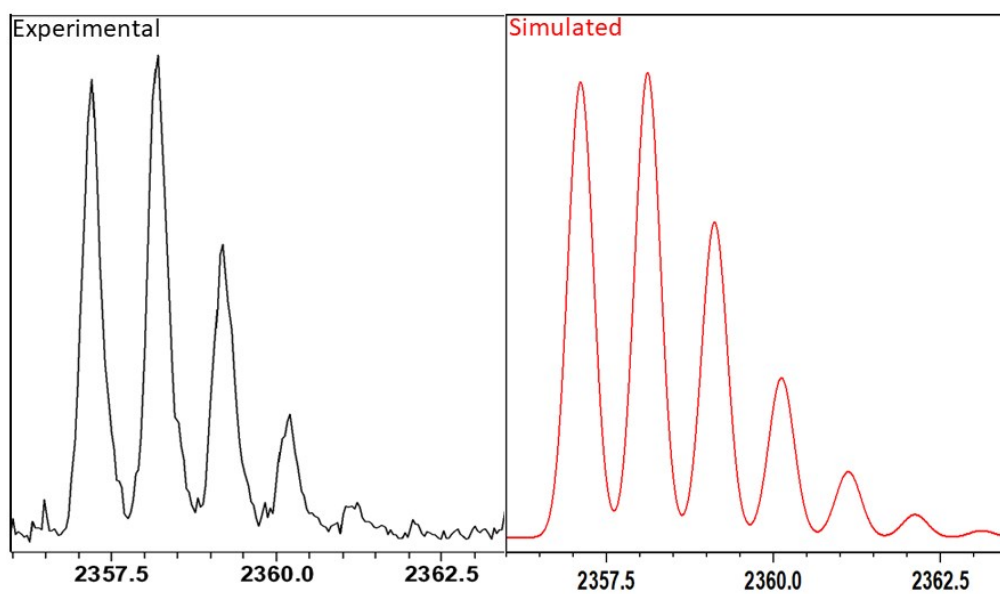


Figure S2 Zoom scan of $[1+Au]^+$ cluster peak (left) and simulated isotope distribution (right)

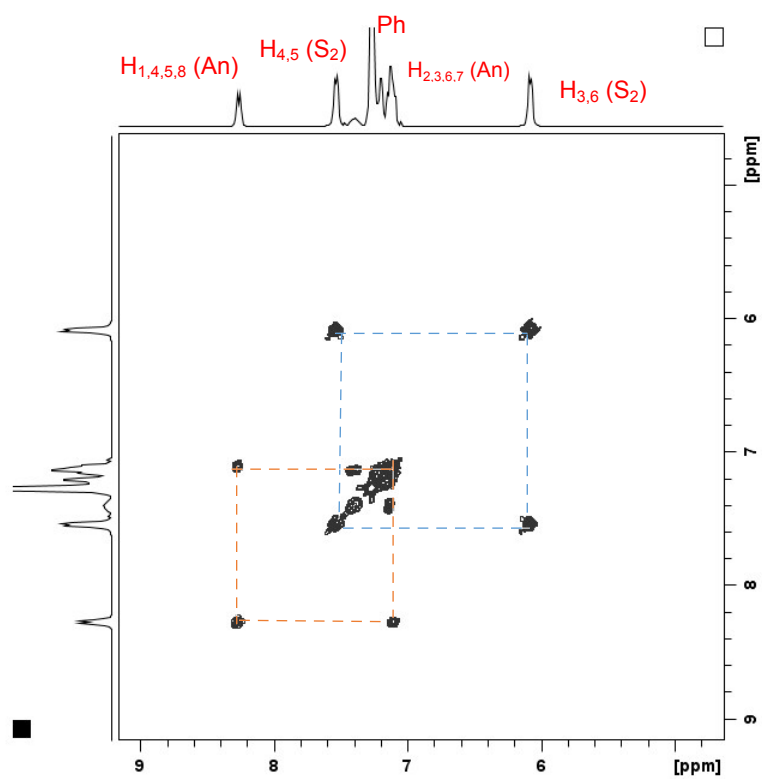


Figure S3 COSY ^1H NMR spectrum of **1** (CDCl_3 , 298 K).

13C AVNEO500 11 July 2021
AuS4 in CDCl3

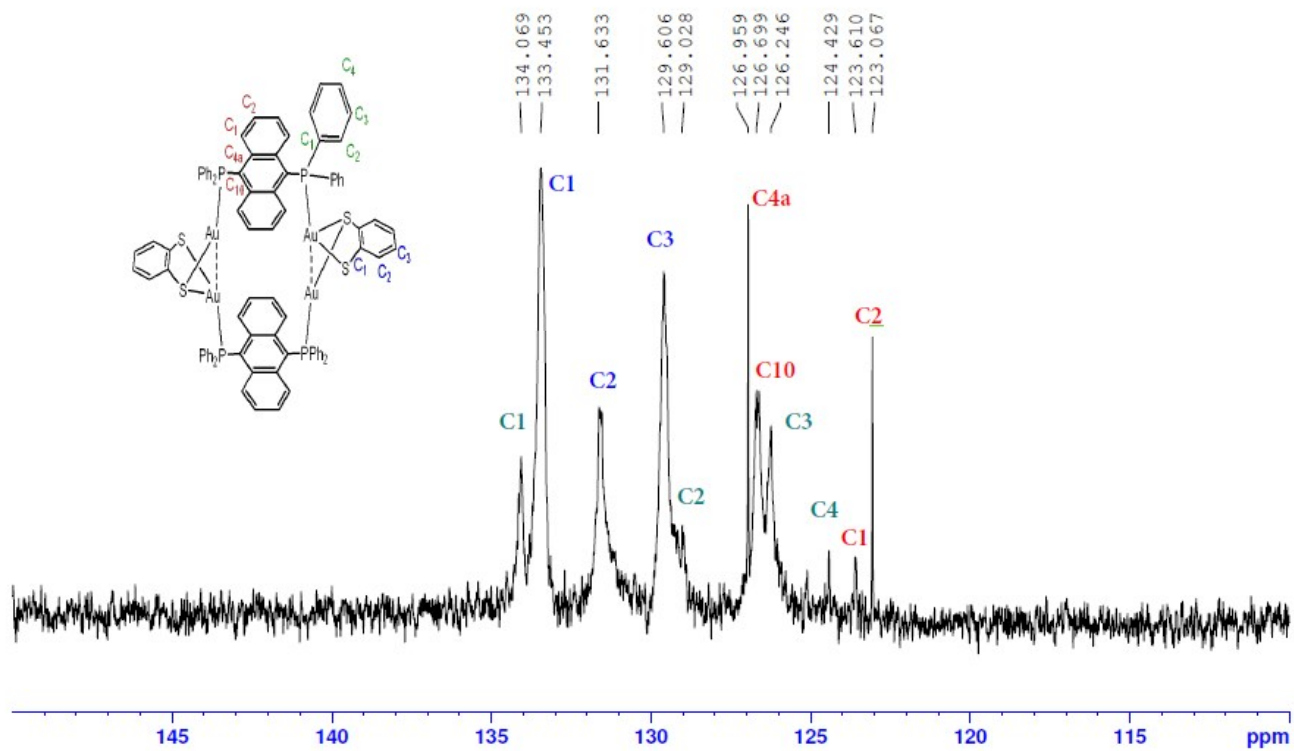


Figure S4 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1** (CDCl_3 , 298 K).

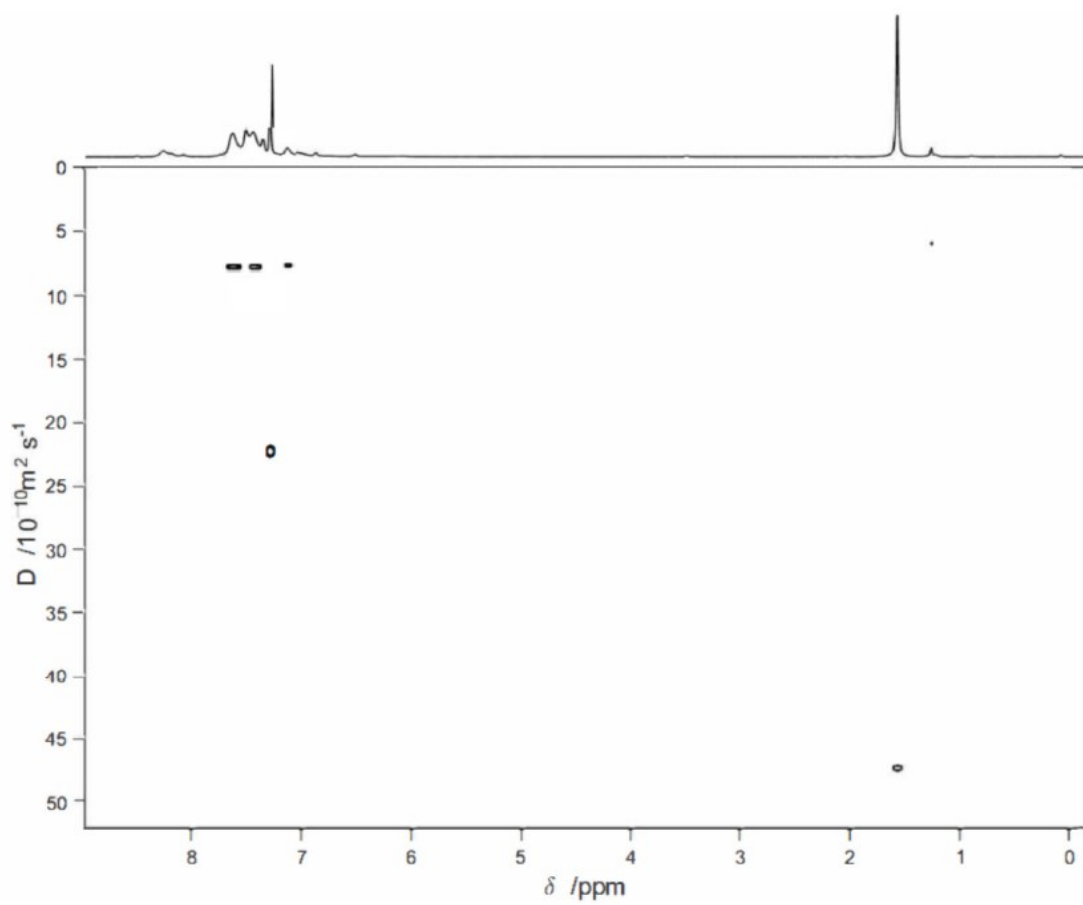


Figure S5 ¹H DOSY NMR spectrum of **1** (CDCl₃, 298 K)