

Electronic Supplementary Materials for

Structural Transformation of Metastable Two-Electron Superatom Au-Doped Cu-Rich Alloy Nanocluster

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Tel.: +886-3-890-3607 (C.W.L.)

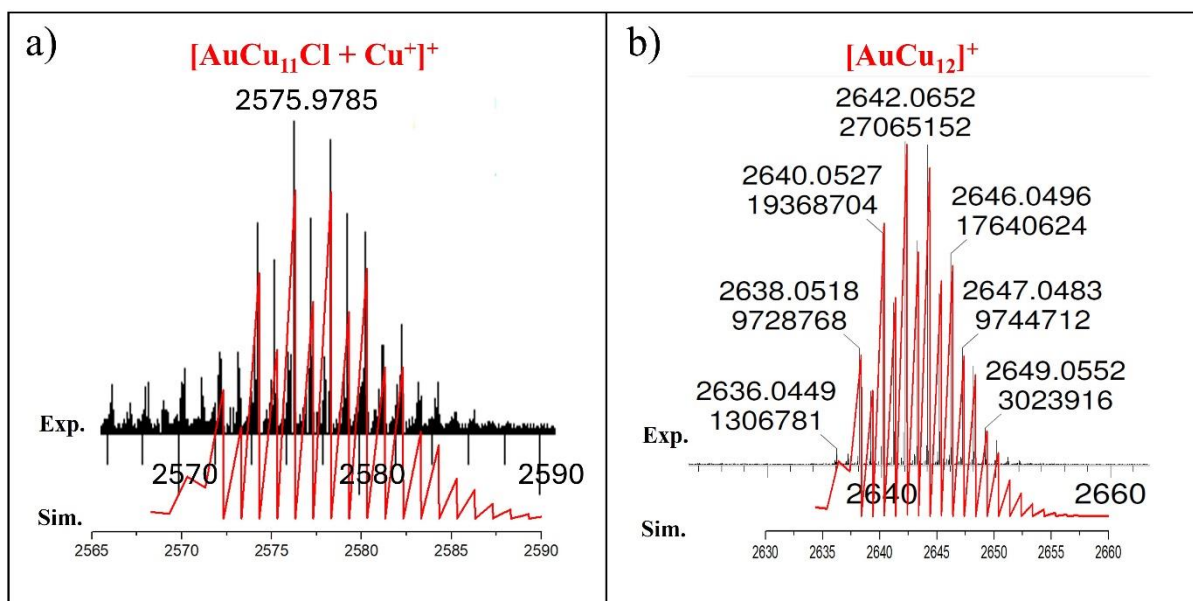


Figure S1. Comparison between the experimental data (top) and the simulated (bottom) isotope patterns of peaks (a) $[\text{AuCu}_{11}\text{Cl} + \text{Cu}^+]^+$ and (b) $[\text{AuCu}_{12}]^+$.

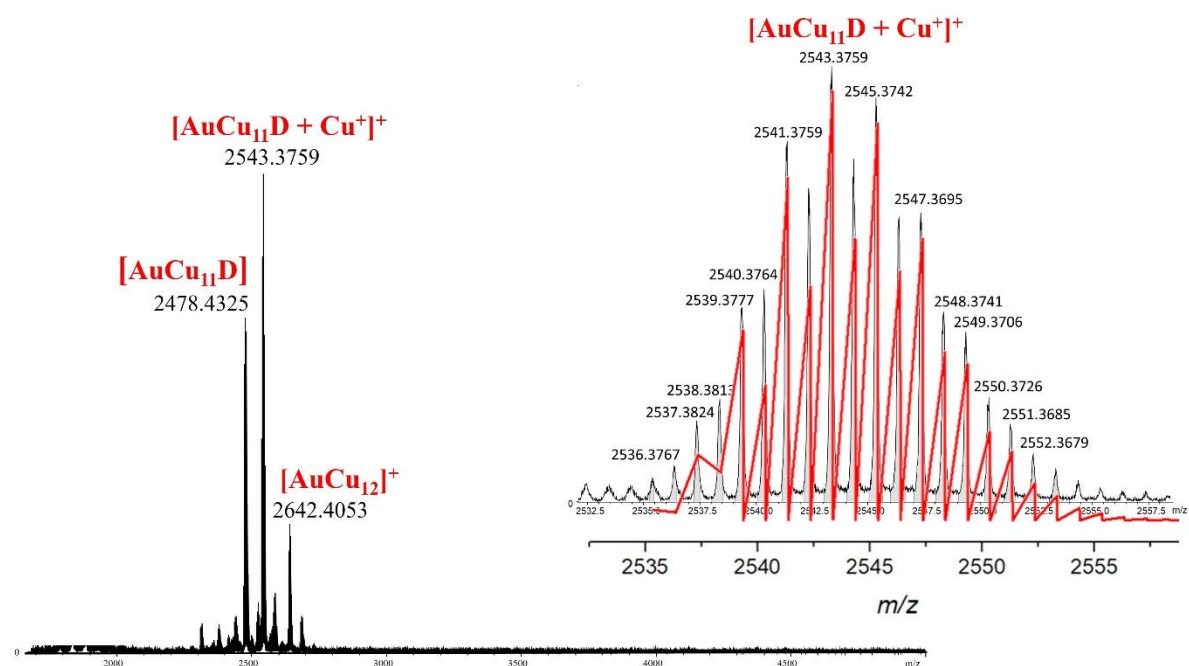


Figure S2. ESI-MS spectra $[\text{AuCu}_{11}\text{D} + \text{Cu}^+]^+$. The insets show the comparisons between the experimental data (top) and the simulated (bottom) isotope patterns for $[\text{AuCu}_{11}\text{D} + \text{Cu}^+]^+$.

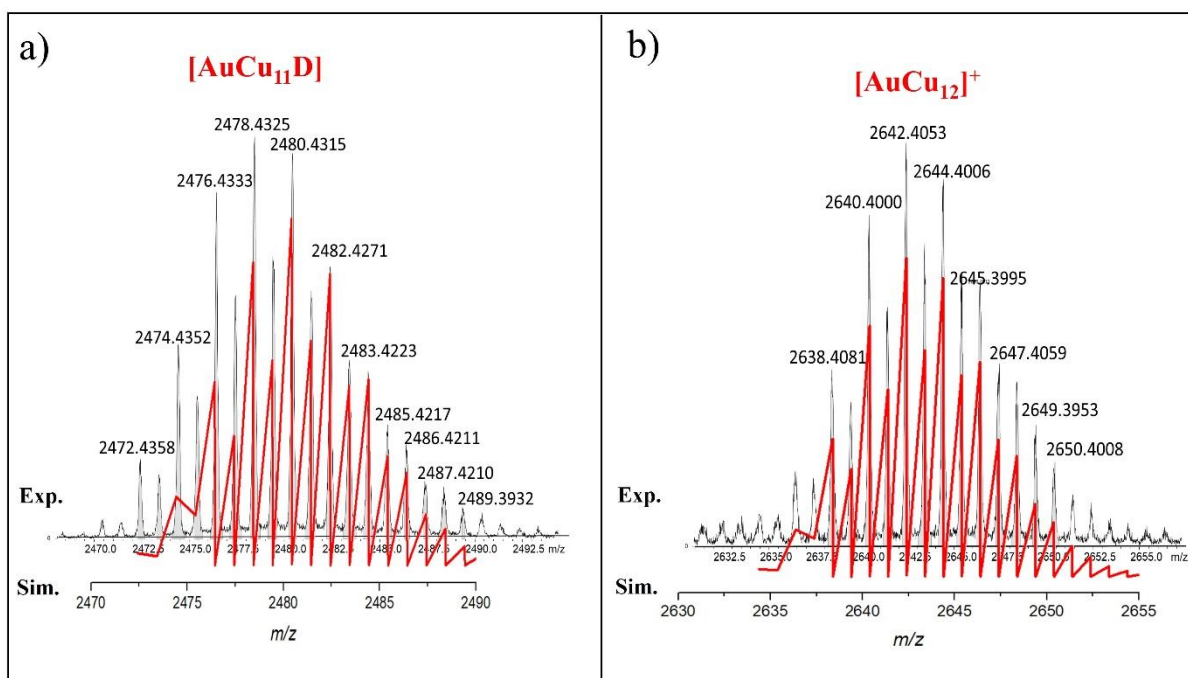


Figure S3. Comparisons between the experimental data (top) and the simulated (bottom) isotope patterns of peaks (a) [AuCu₁₁D] and (b) [AuCu₁₂]⁺.

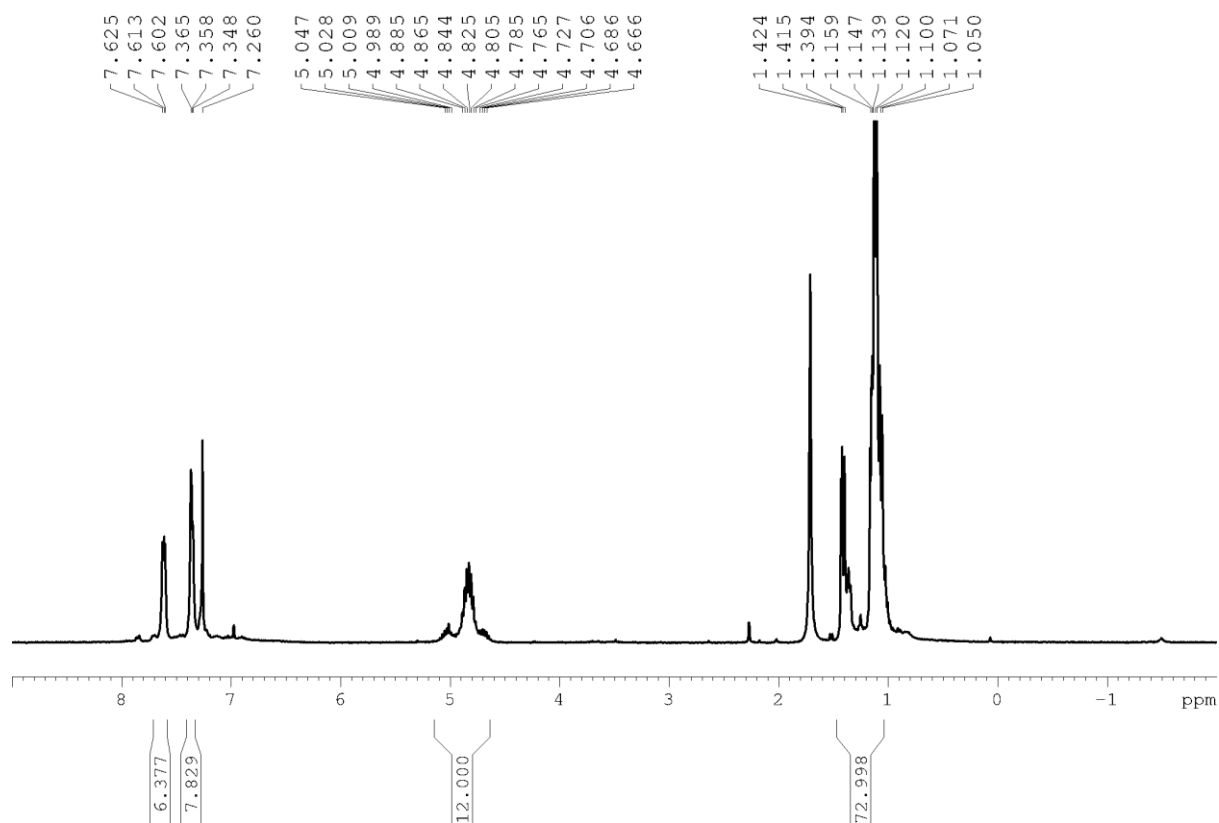


Figure S4. ¹H NMR spectrum of AuCu₁₁D in CDCl₃.

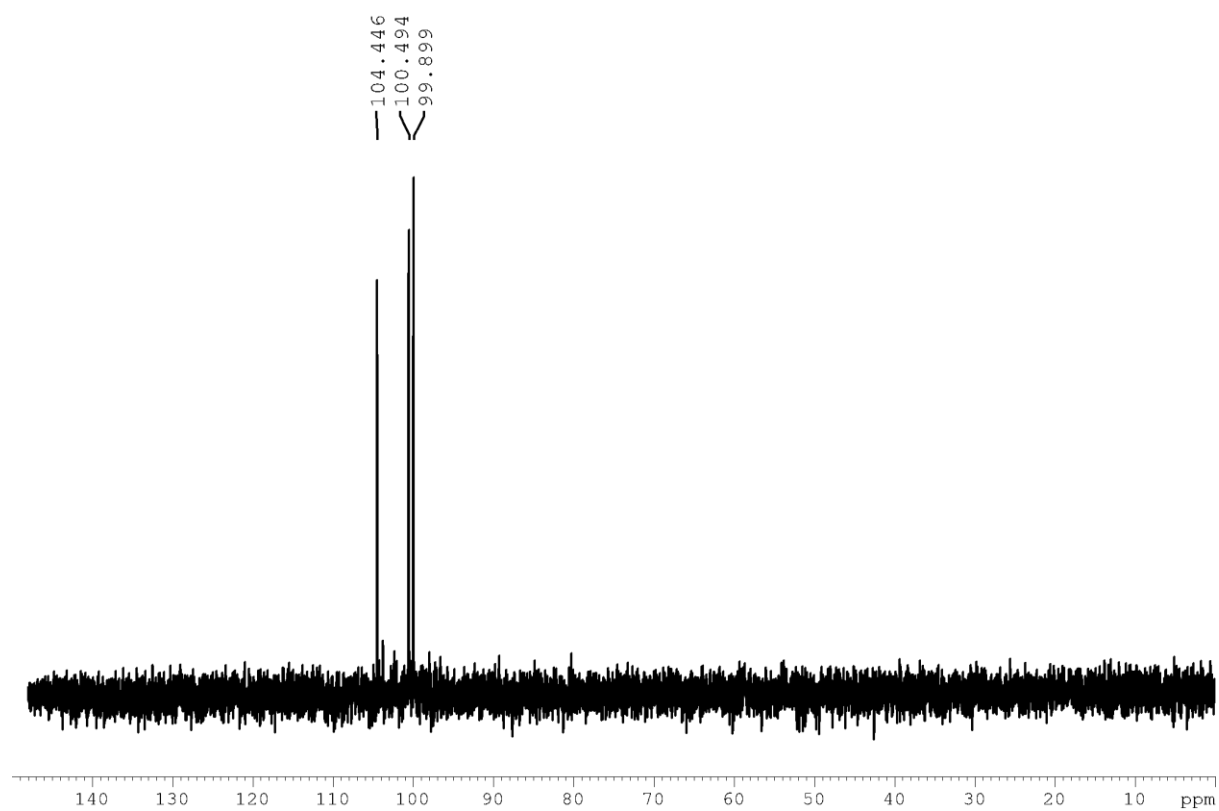


Figure S5. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of AuCu_{11}H in CDCl_3 .

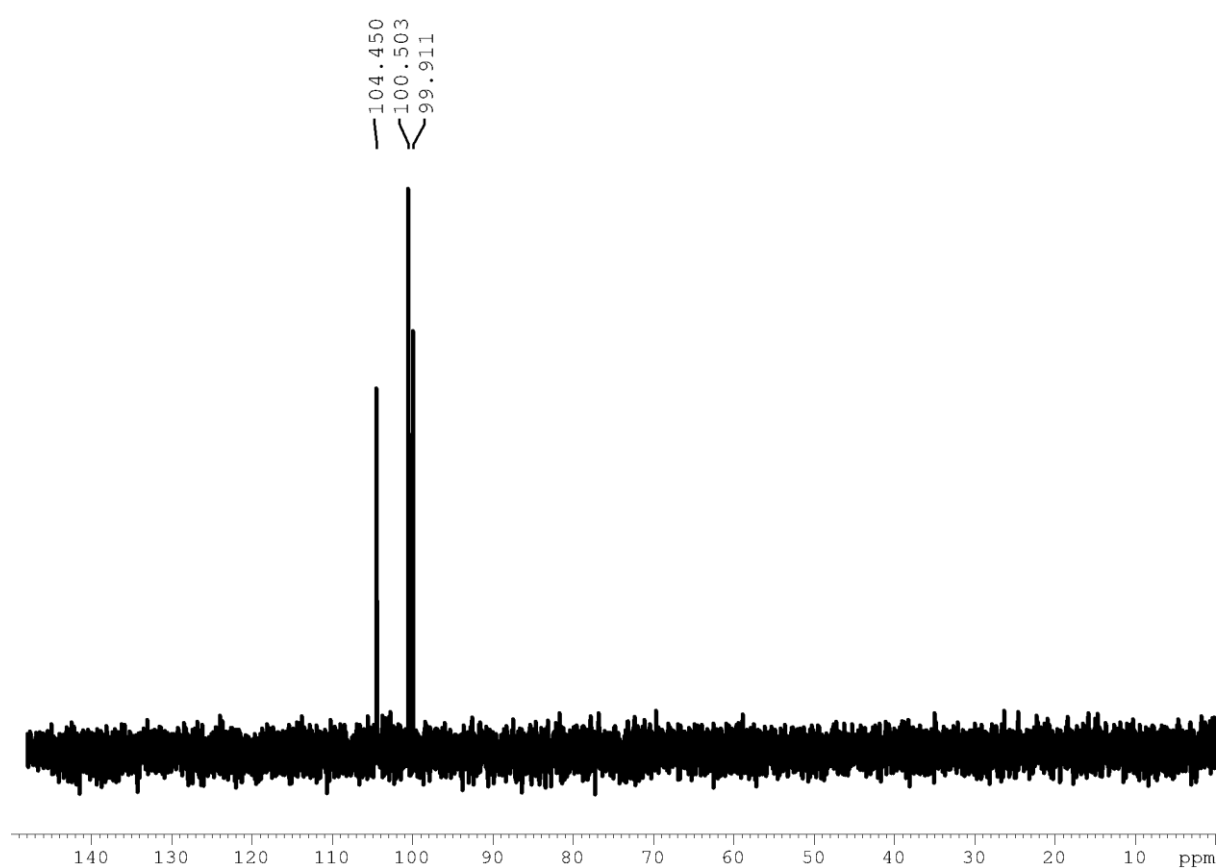


Figure S6. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of AuCu_{11}D in CDCl_3 .

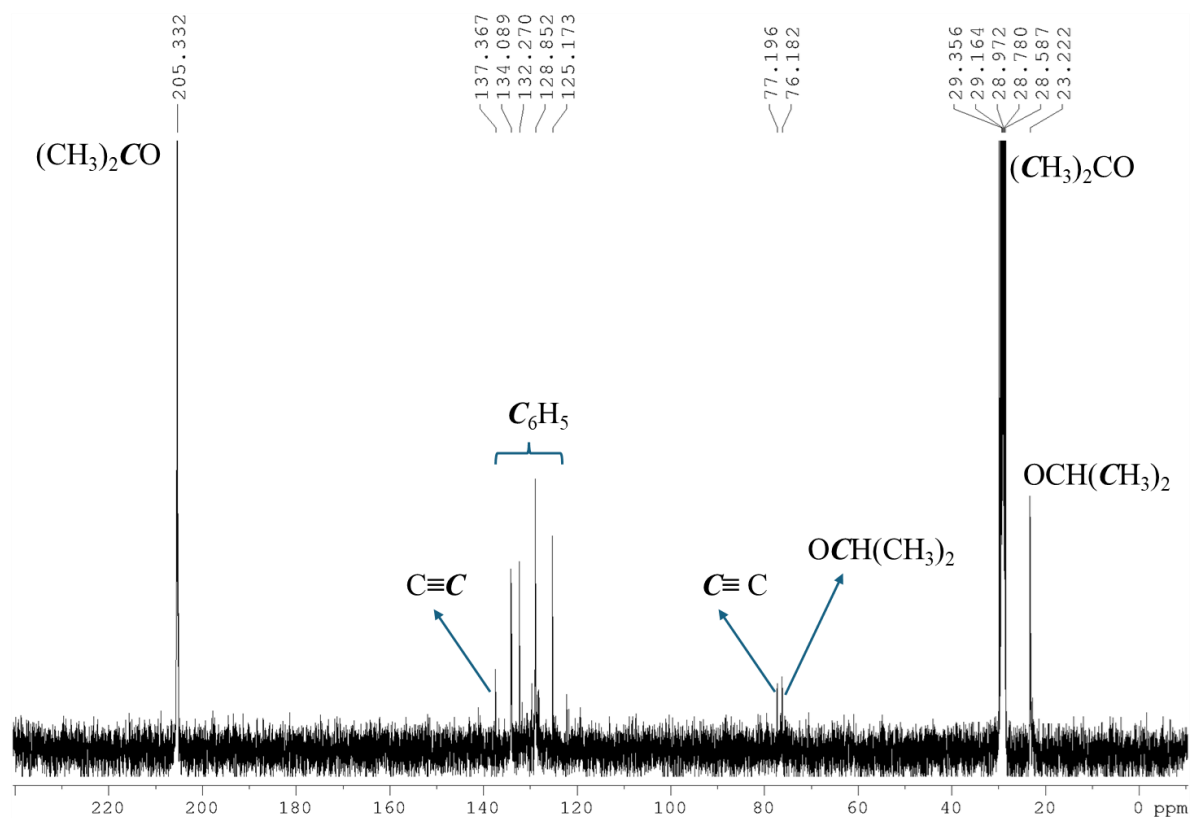


Figure S7. ^{13}C NMR spectrum of AuCu_{11}H in d_6 -acetone.

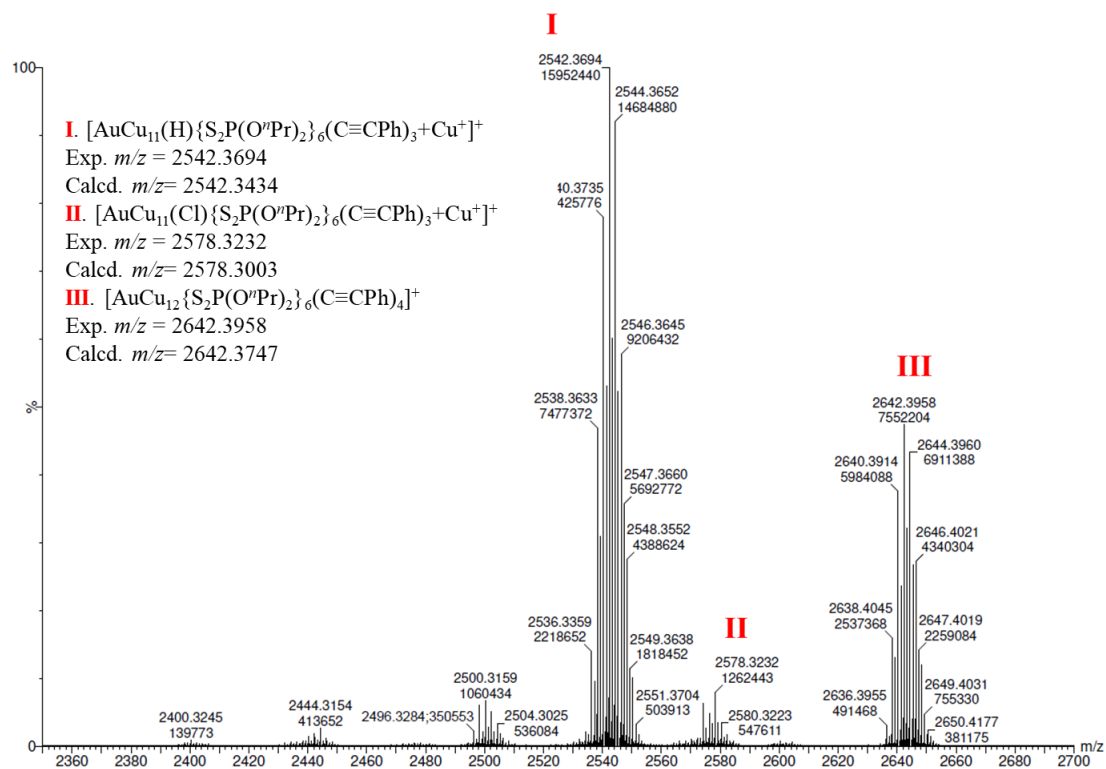


Figure S8. The ESI-MS spectrum of $[\text{AuCu}_{11}(\text{H})\{\text{S}_2\text{P}(\text{O}^i\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_3+\text{Cu}^+]^+$ (I), $[\text{AuCu}_{11}(\text{Cl})\{\text{S}_2\text{P}(\text{O}^i\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_3+\text{Cu}^+]^+$ (II), and $[\text{AuCu}_{12}\{\text{S}_2\text{P}(\text{O}^i\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_4]^+$ (III).

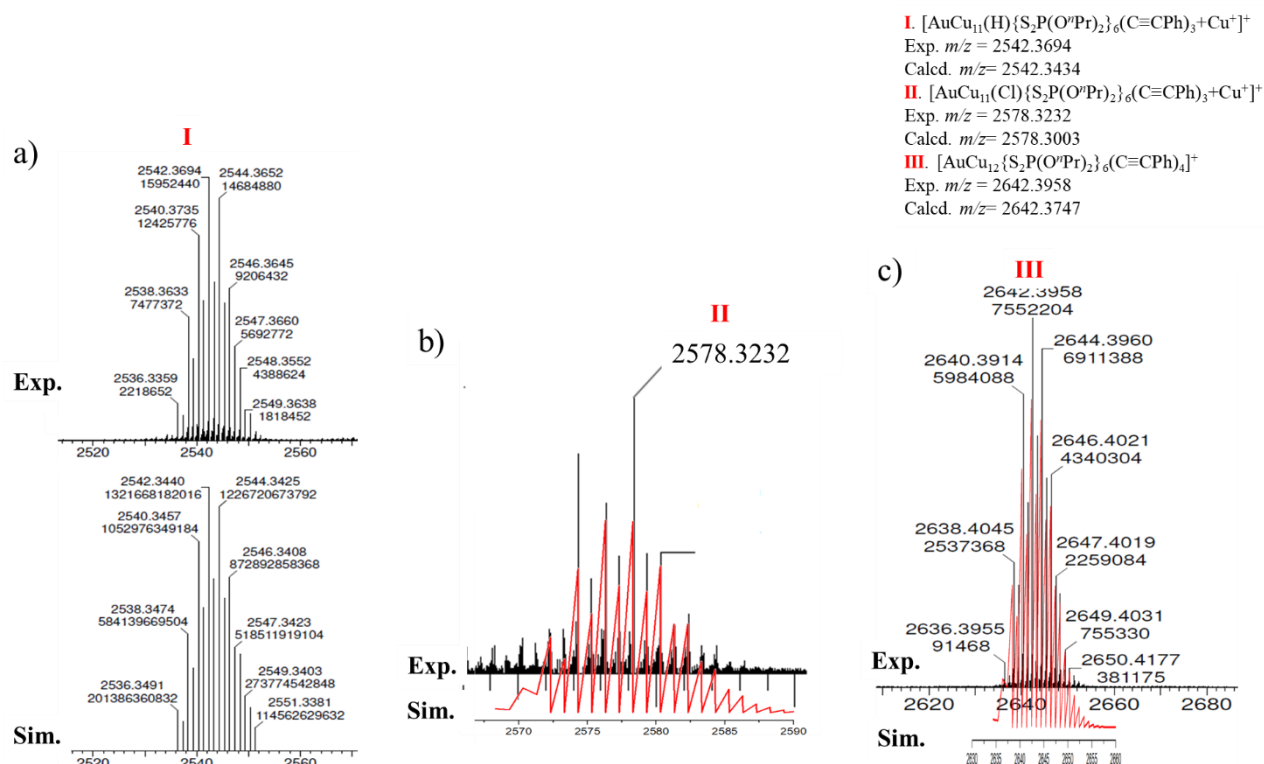


Figure S9. Comparisons between the experimental data (top) and the simulated (bottom) isotope patterns of peaks (a) $[\text{AuCu}_{11}(\text{H})\{\text{S}_2\text{P}(\text{O}^i\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_3+\text{Cu}^+]^+$ (I), (b) $[\text{AuCu}_{11}(\text{Cl})\{\text{S}_2\text{P}(\text{O}^i\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_3+\text{Cu}^+]^+$ (II), and (c) $[\text{AuCu}_{12}\{\text{S}_2\text{P}(\text{O}^i\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_4]^+$ (III).

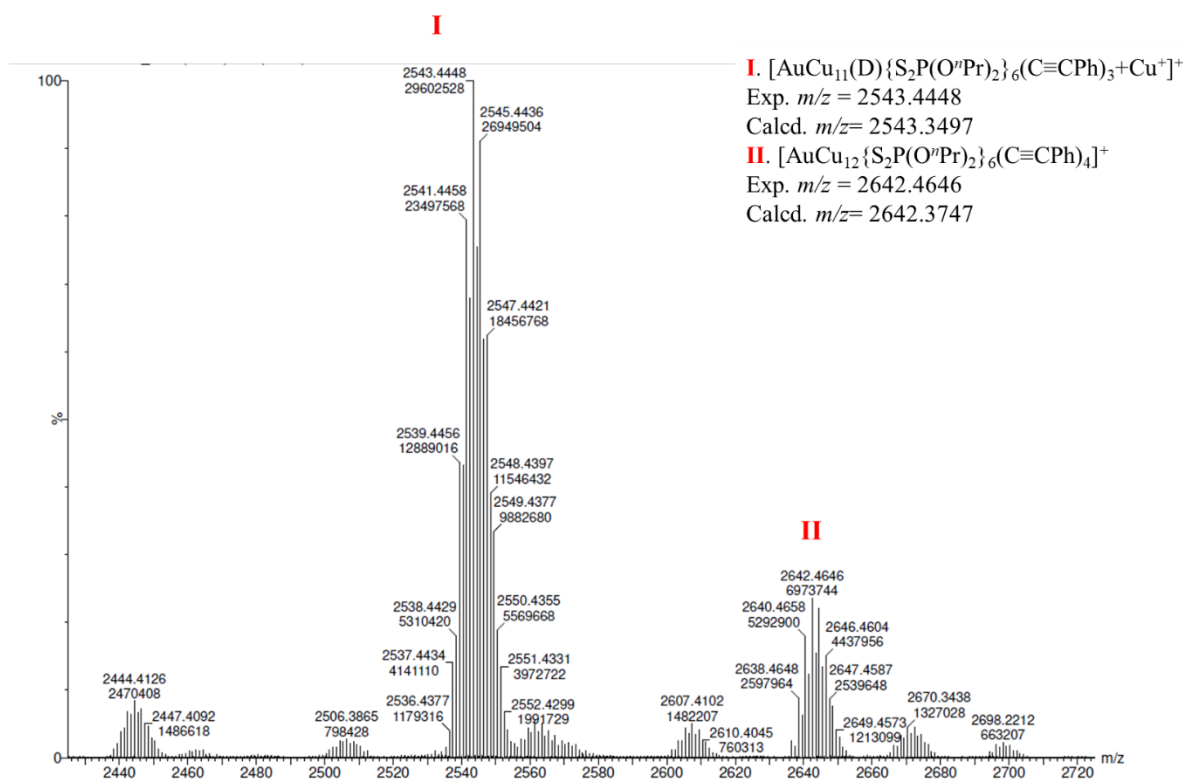
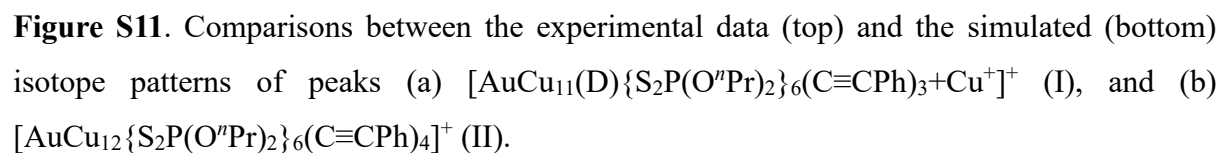


Figure S10. The ESI-MS spectrum of $[\text{AuCu}_{11}(\text{D})\{\text{S}_2\text{P}(\text{O}''\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_3+\text{Cu}^+]^+$ (I), and $[\text{AuCu}_{12}\{\text{S}_2\text{P}(\text{O}''\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_4]^+$ (II).

b)



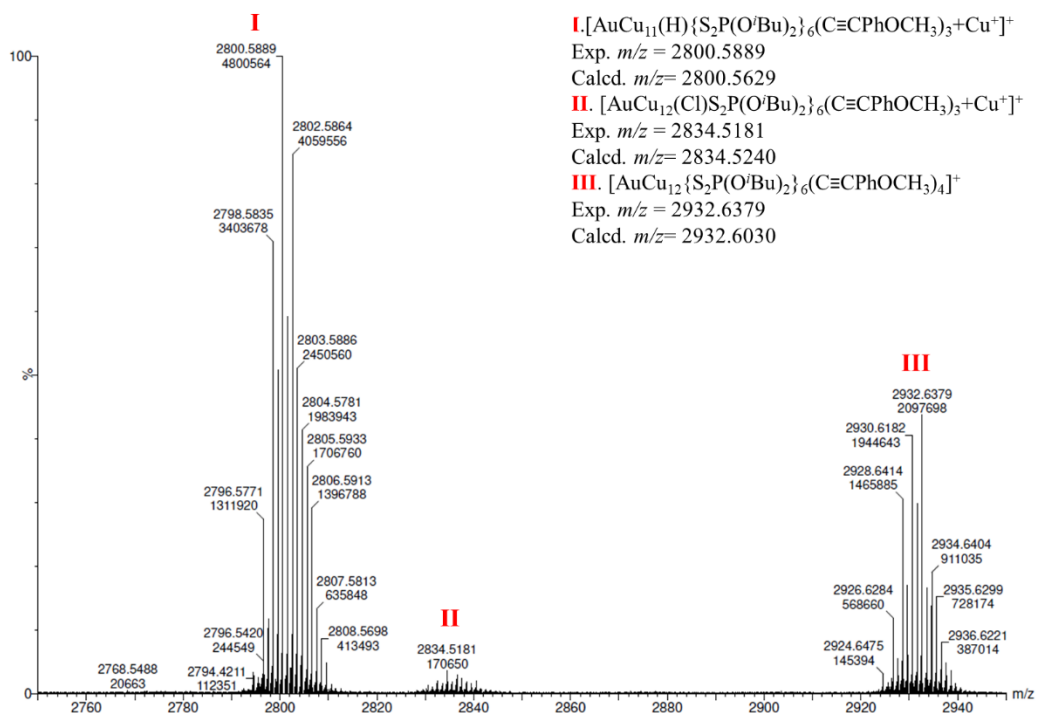


Figure S12. The ESI-MS spectrum of $[\text{AuCu}_{11}(\text{H})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3+\text{Cu}^+]^+$ (I), $[\text{AuCu}_{11}(\text{Cl})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3+\text{Cu}^+]^+$ (II), and $[\text{AuCu}_{12}\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_4]^+$ (III).

I. $[\text{AuCu}_{11}(\text{H})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3+\text{Cu}^+]^+$
 Exp. $m/z = 2800.5889$
 Calcd. $m/z = 2800.5629$
II. $[\text{AuCu}_{12}(\text{Cl})\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3+\text{Cu}^+]^+$
 Exp. $m/z = 2834.5181$
 Calcd. $m/z = 2834.5240$
III. $[\text{AuCu}_{12}\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_4]^+$
 Exp. $m/z = 2932.6379$
 Calcd. $m/z = 2932.6030$

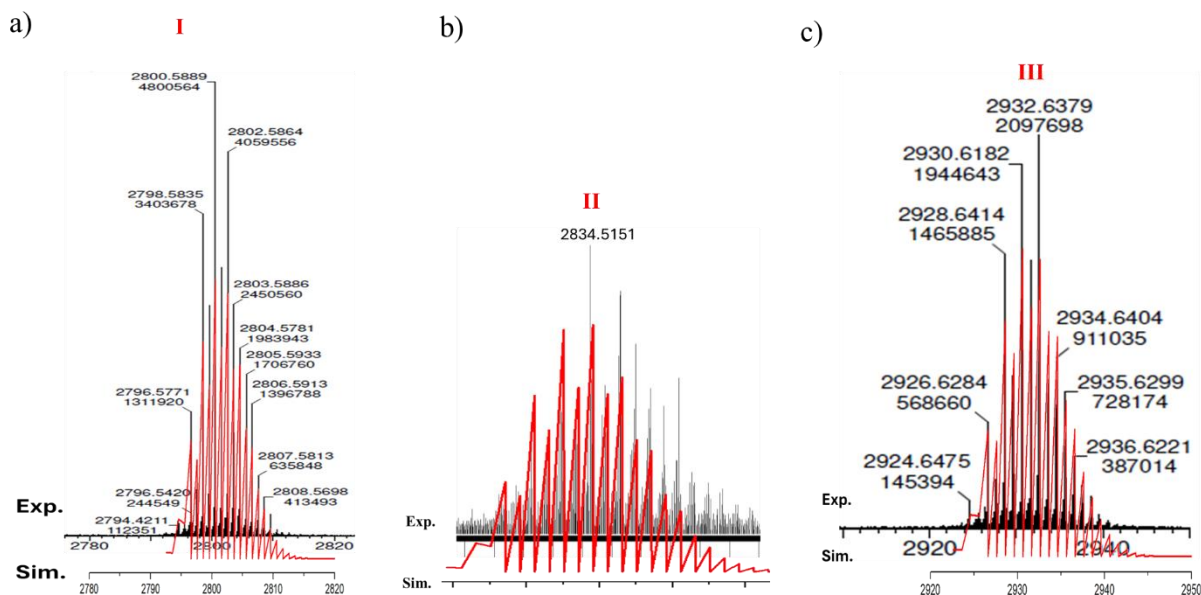


Figure S13. Comparisons between the experimental data (top) and the simulated (bottom) isotope patterns of peaks (a) $[\text{AuCu}_{11}(\text{H})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3+\text{Cu}^+]^+$ (I), (b) $[\text{AuCu}_{11}(\text{Cl})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3+\text{Cu}^+]^+$ (II), and (c) $[\text{AuCu}_{12}\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_4]^+$ (II).

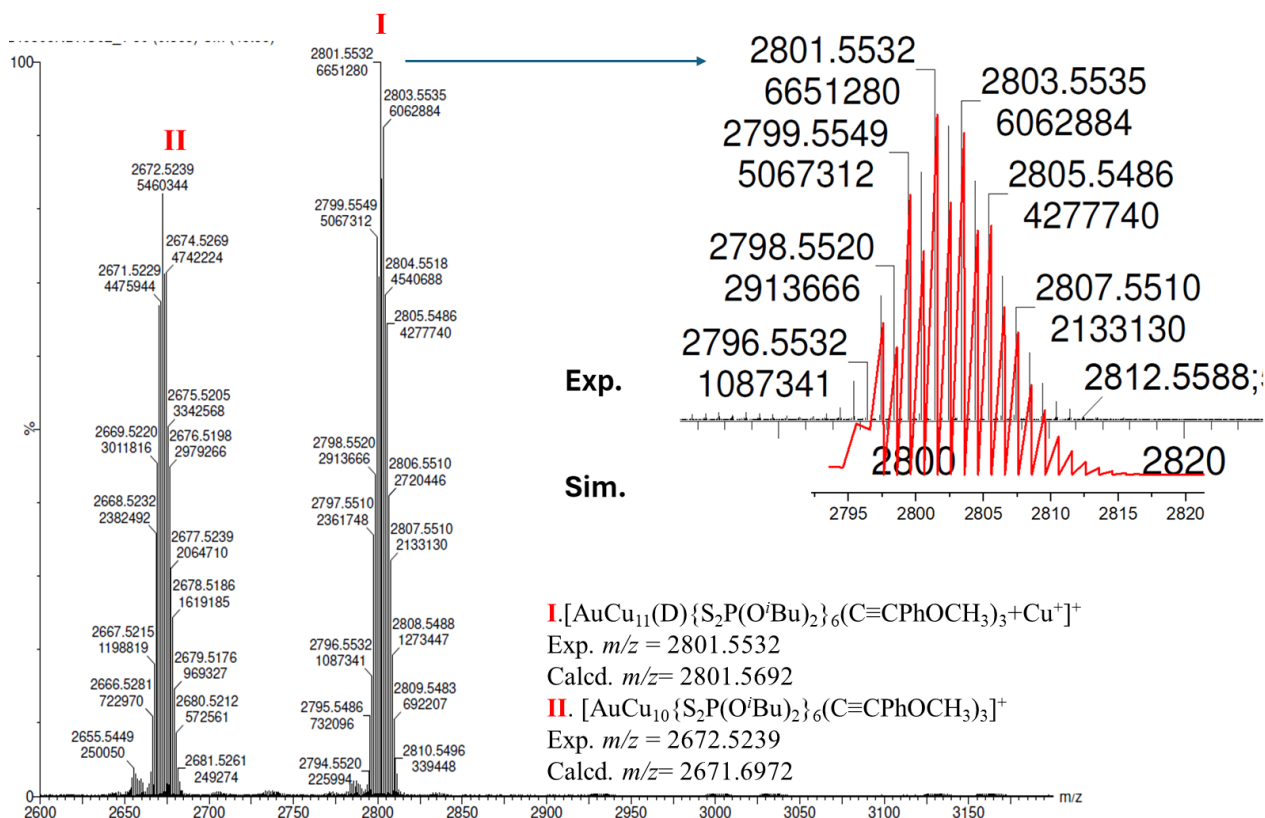


Figure S14. The ESI-MS spectrum of $[\text{AuCu}_{11}(\text{D})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3+\text{Cu}^+]^+$ (I), and $[\text{AuCu}_{10}\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3]^+$ (II). Inset: Comparisons between the experimental data (top) and the simulated (bottom) isotope pattern of peaks $[\text{AuCu}_{11}(\text{D})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3+\text{Cu}^+]^+$ (I).

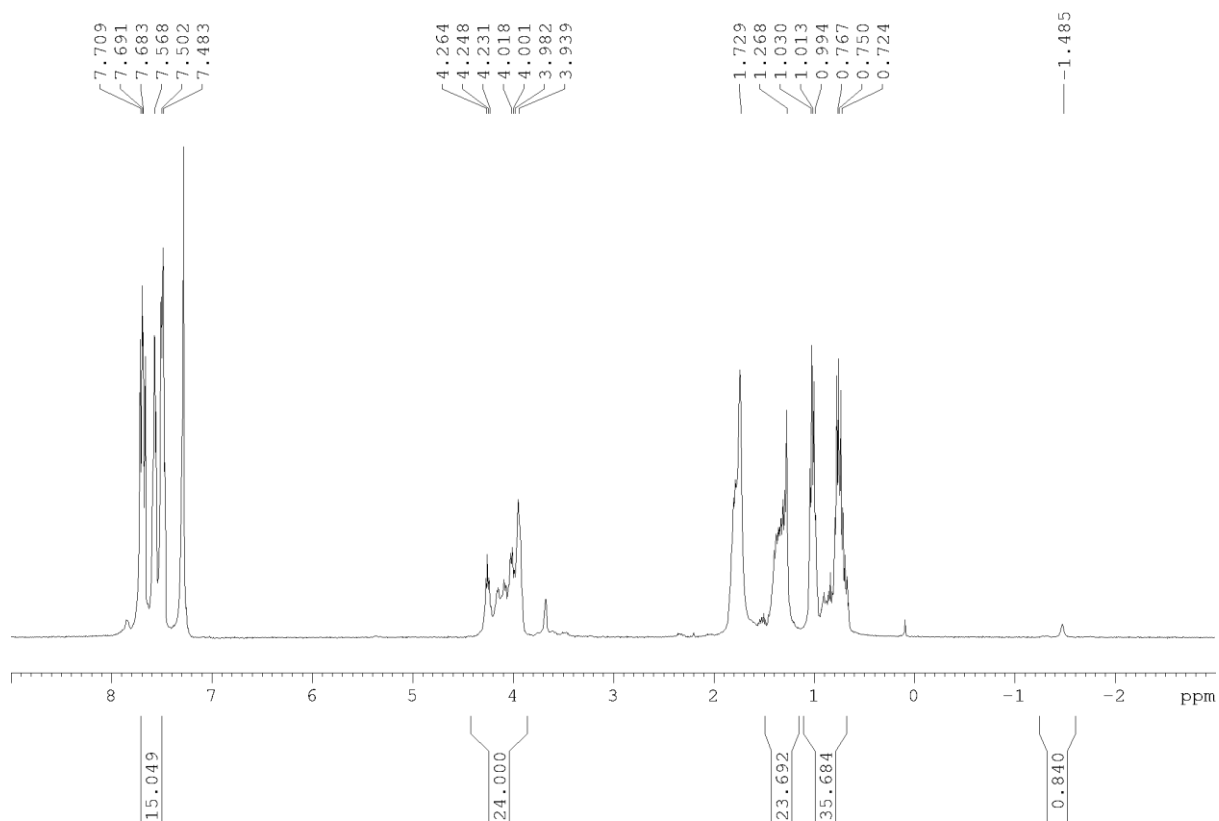


Figure S15. ¹H NMR spectrum of [AuCu₁₁(H){S₂P(O^{*i*}Pr)₂}₆(C≡CPh)₃] in CDCl₃.

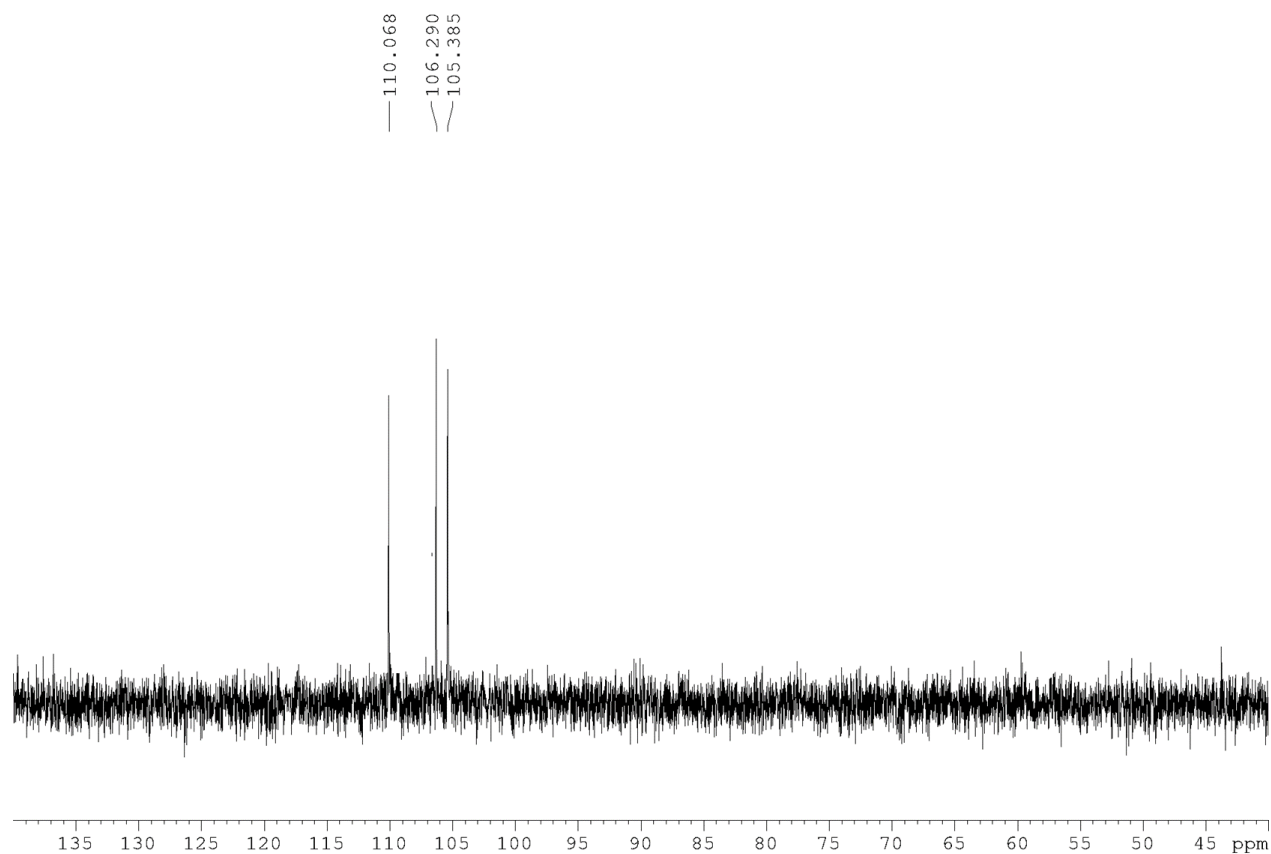


Figure S16. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{AuCu}_{11}(\text{H})\{\text{S}_2\text{P}(\text{O}^i\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_3]$ in CDCl_3 .

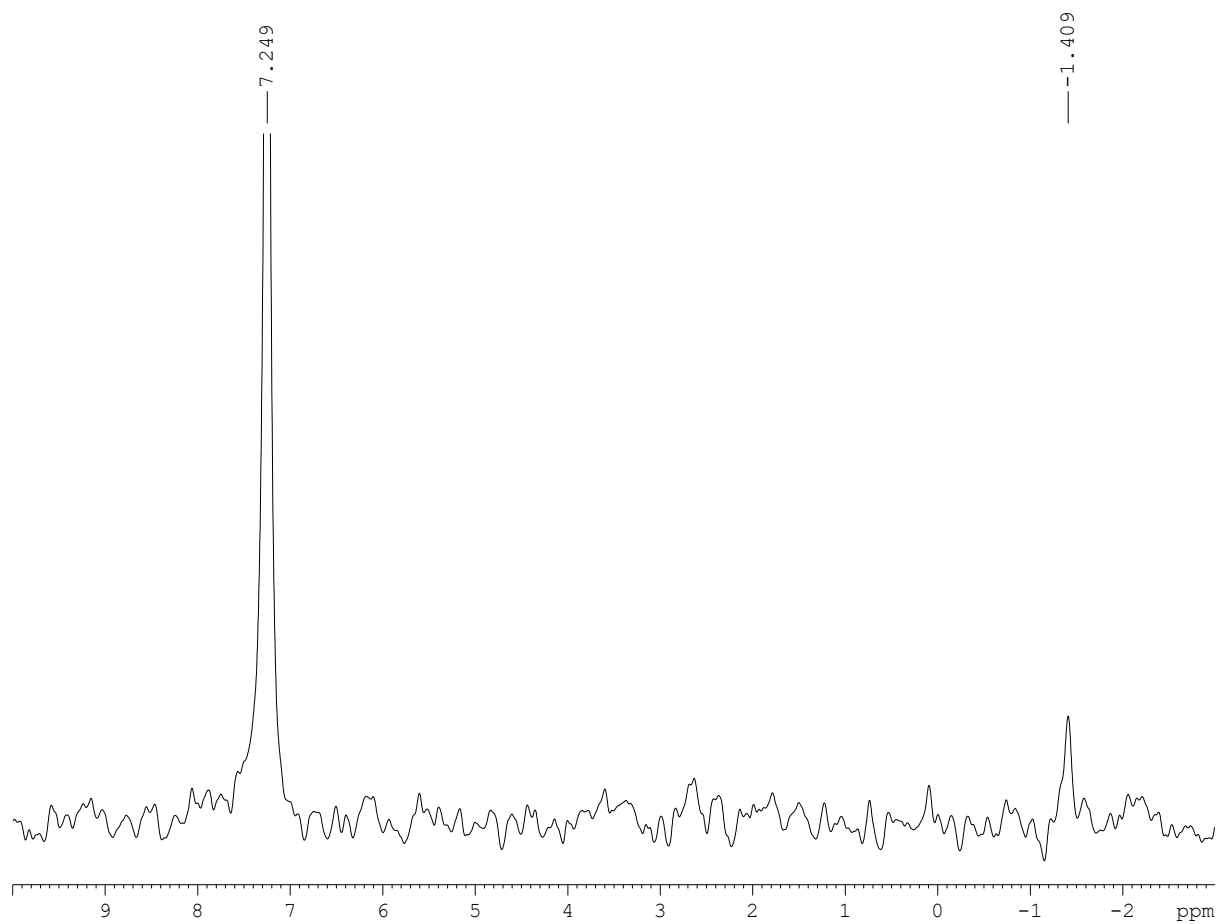


Figure S17. ^2H NMR spectrum of $[\text{AuCu}_{11}(\text{D})\{\text{S}_2\text{P}(\text{O}^i\text{Pr})_2\}_6(\text{C}\equiv\text{CPh})_3]$ in CHCl_3 .

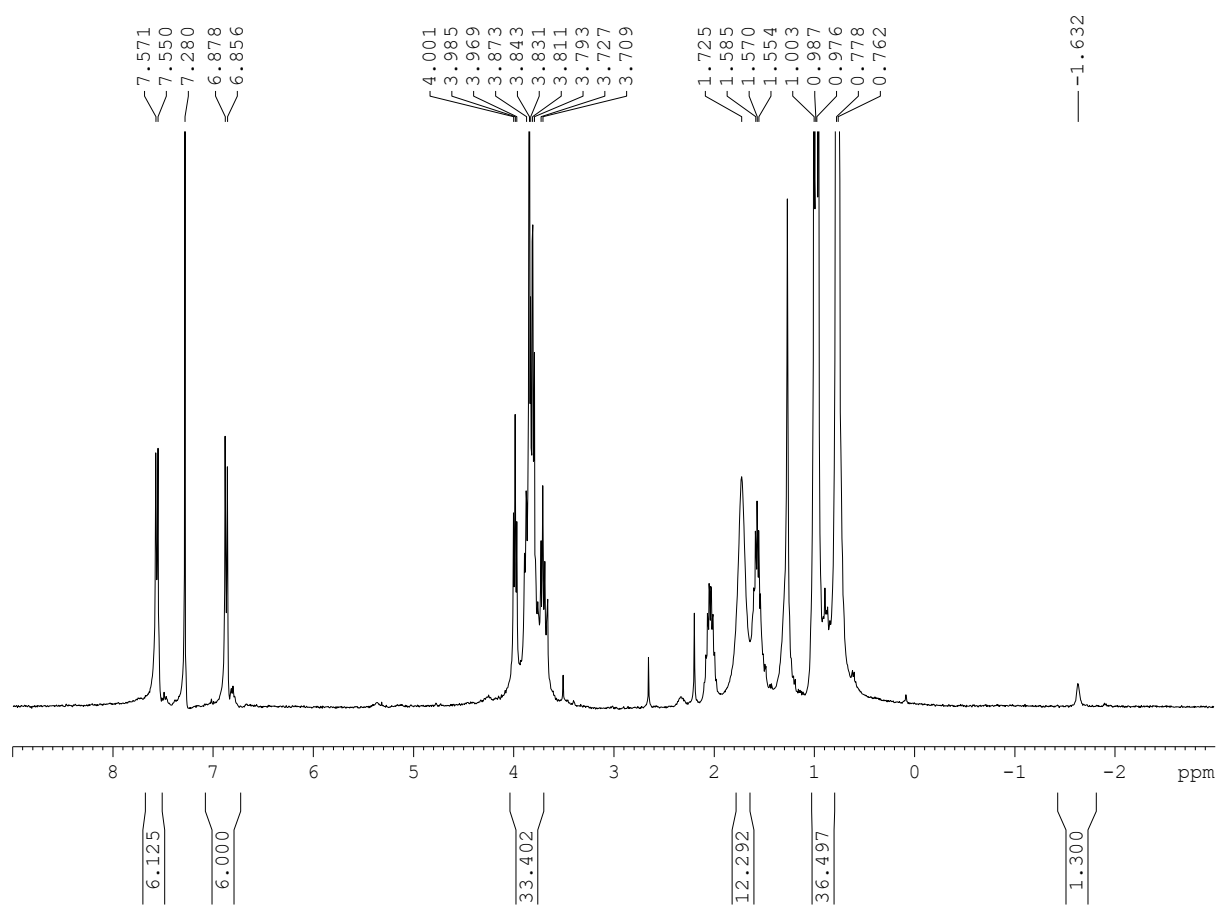


Figure S18. ^1H NMR spectrum of $[\text{AuCu}_{11}(\text{H})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3]$ in CDCl_3 .

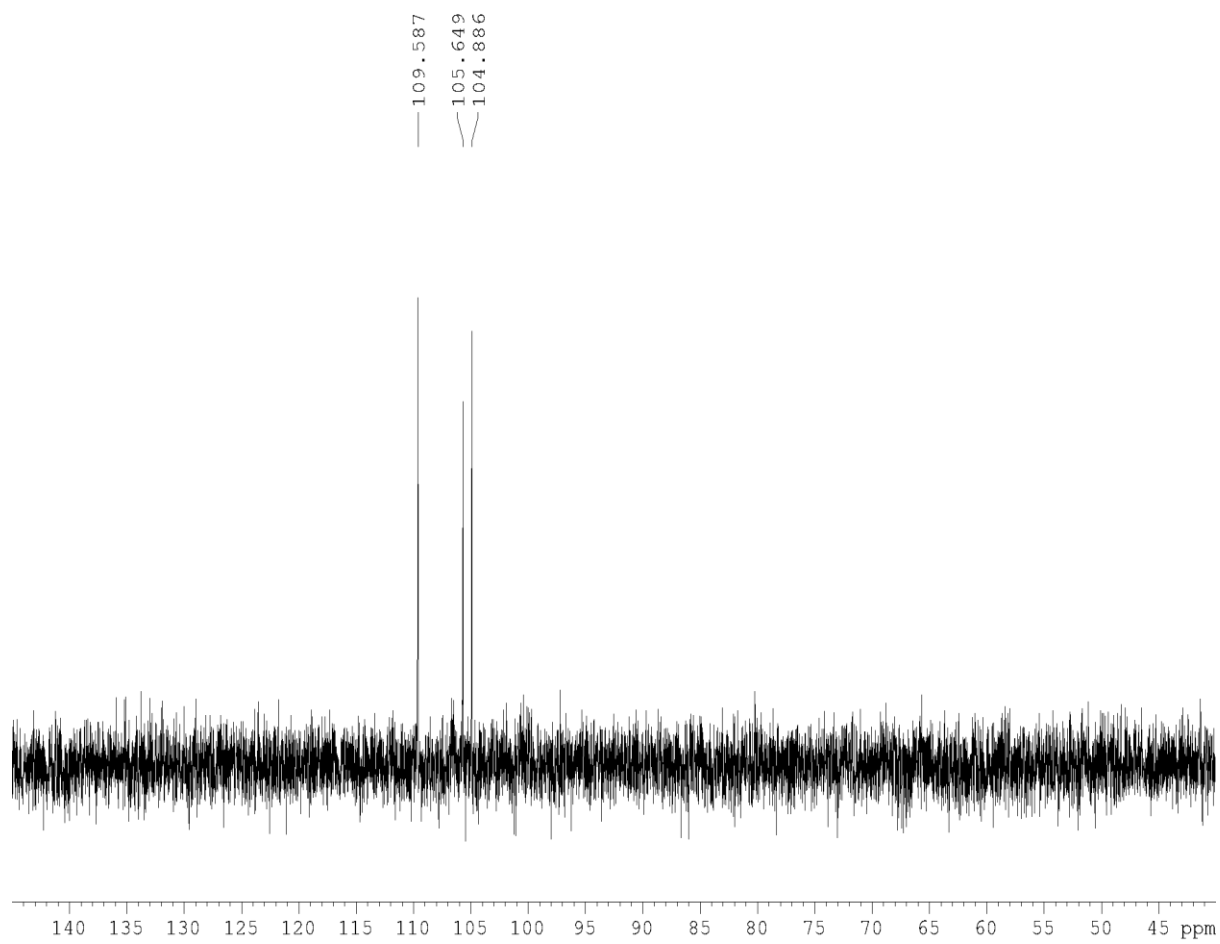


Figure S19. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{AuCu}_{11}(\text{H})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3]$ in CDCl_3 .

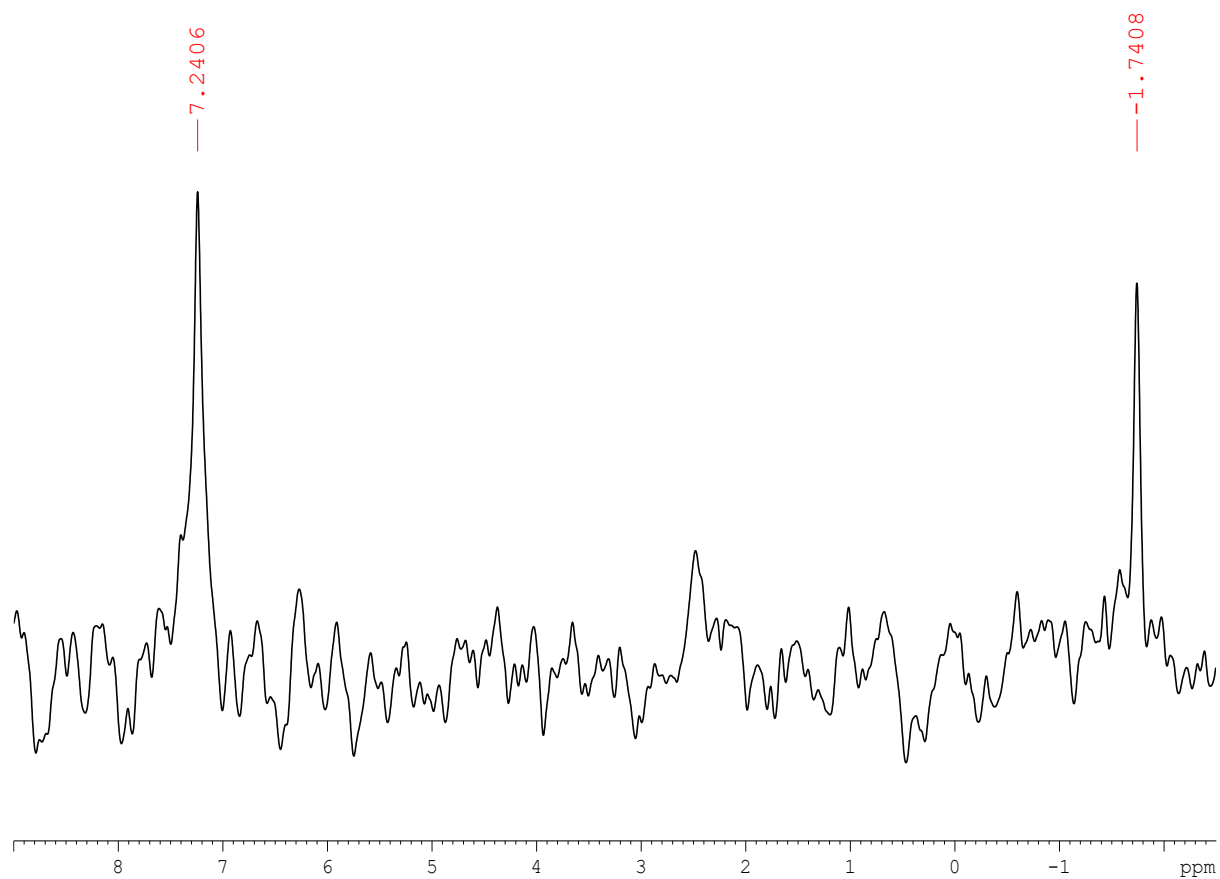


Figure S20. ^2H NMR spectrum of $[\text{AuCu}_{11}(\text{D})\{\text{S}_2\text{P}(\text{O}^i\text{Bu})_2\}_6(\text{C}\equiv\text{CPhOCH}_3)_3]$ in CHCl_3 .

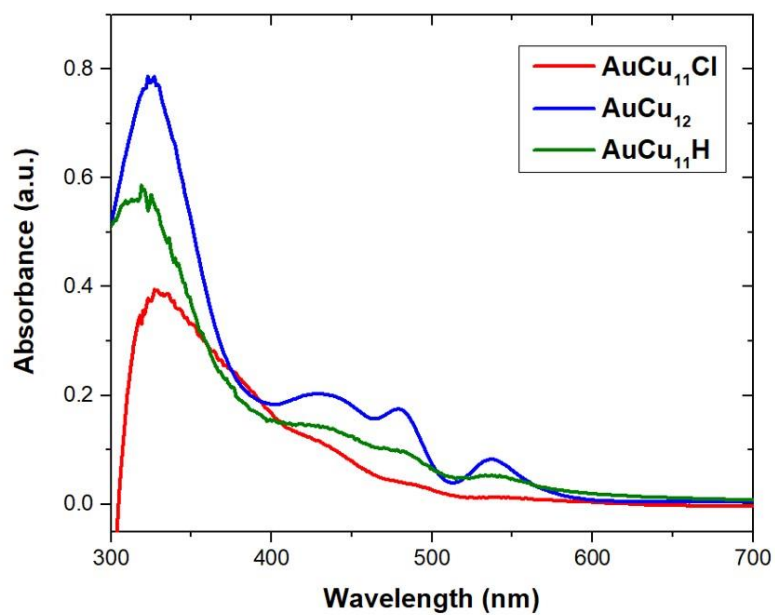


Figure S21. Comparison of the UV-vis absorption spectra of AuCu_{11}H , $\text{AuCu}_{11}\text{Cl}$ and AuCu_{12} in 2-MeTHF solution.

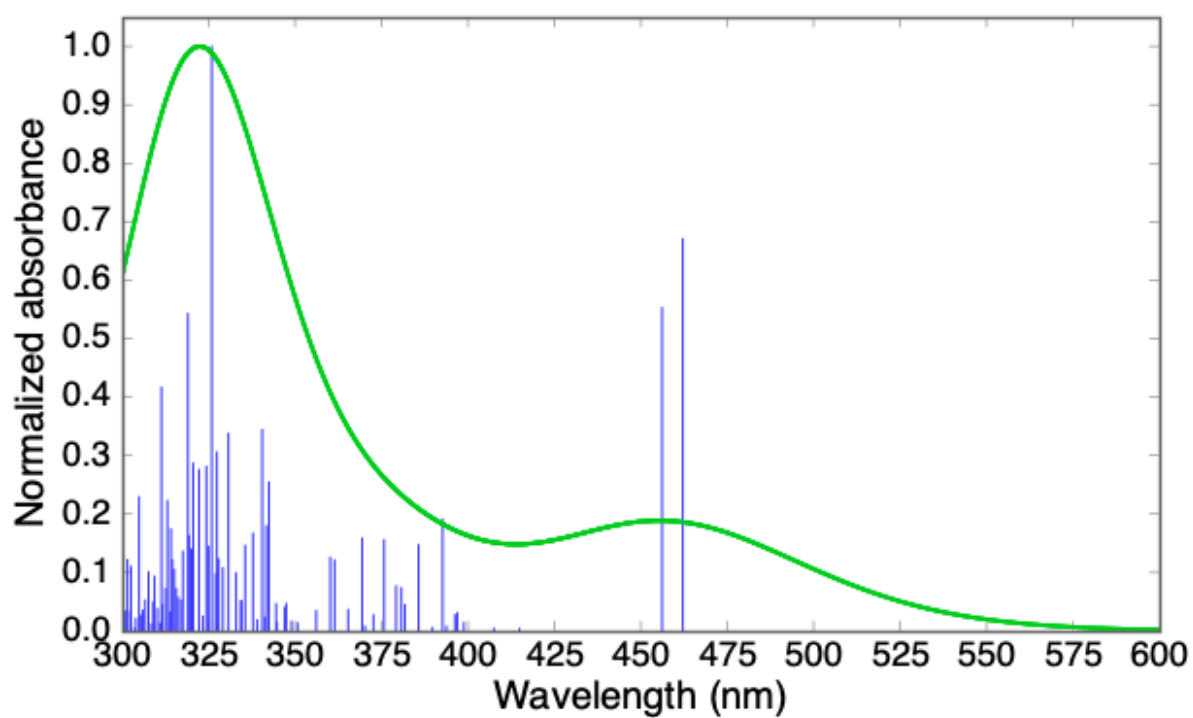


Figure S22. The TD-DFT-simulated UV-vis spectrum of **AuCu₁₁H**, with individual transitions as vertical bars of lengths proportional to their oscillator strengths.

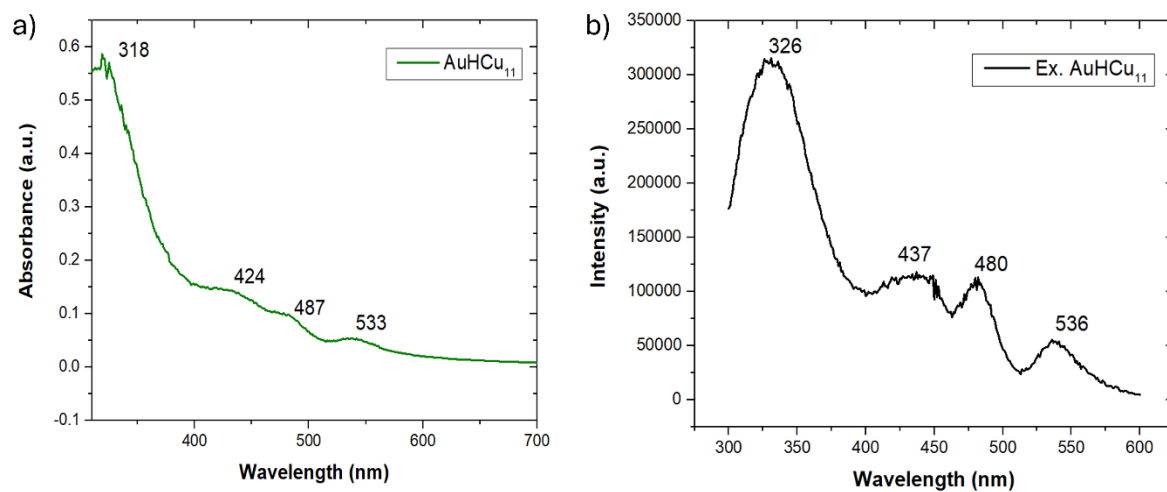


Figure S23. (a) The UV-vis absorption spectrum of **AuCu₁₁H**. (b) The excitation spectrum of **AuCu₁₁H** in 2-MeTHF solution at ambient temperature.

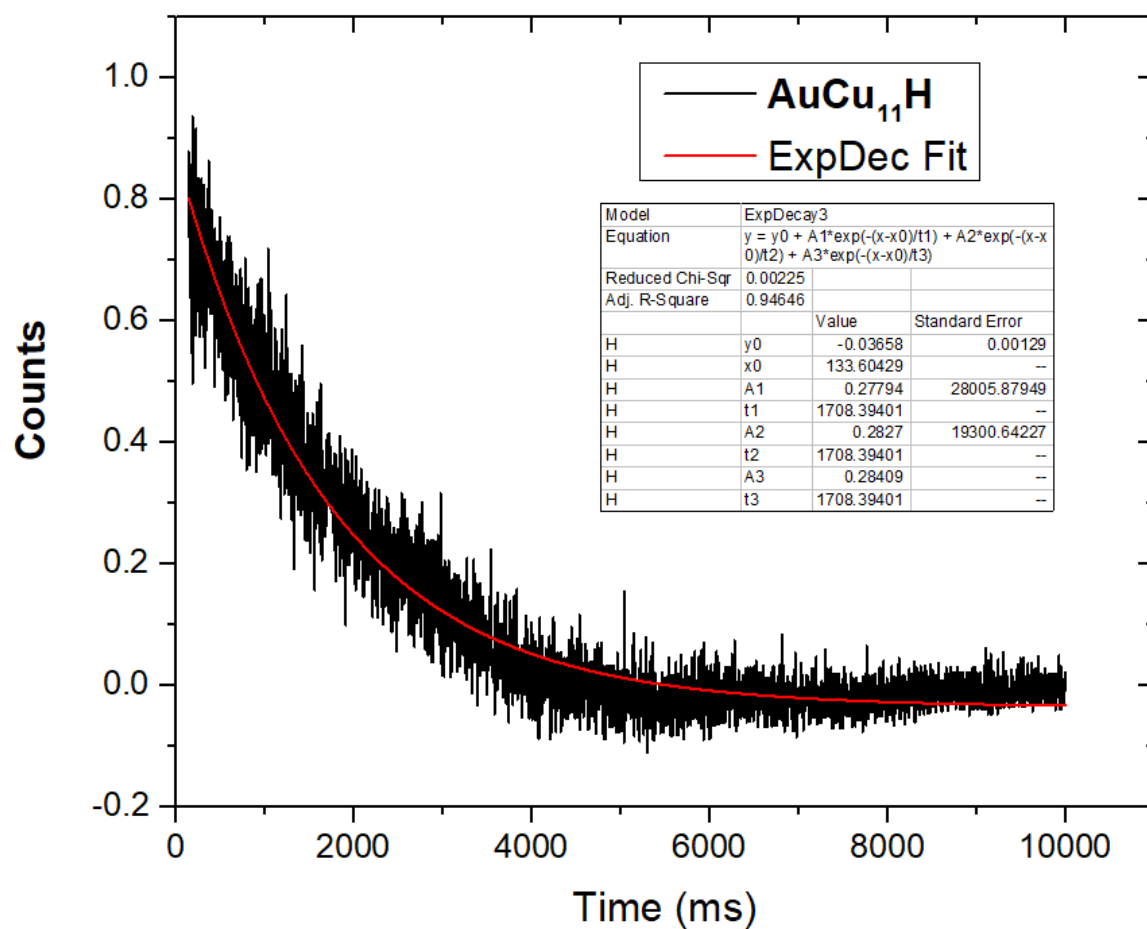


Figure S24. The Emission lifetime of cluster **AuCu₁₁H** at ambient temperature.

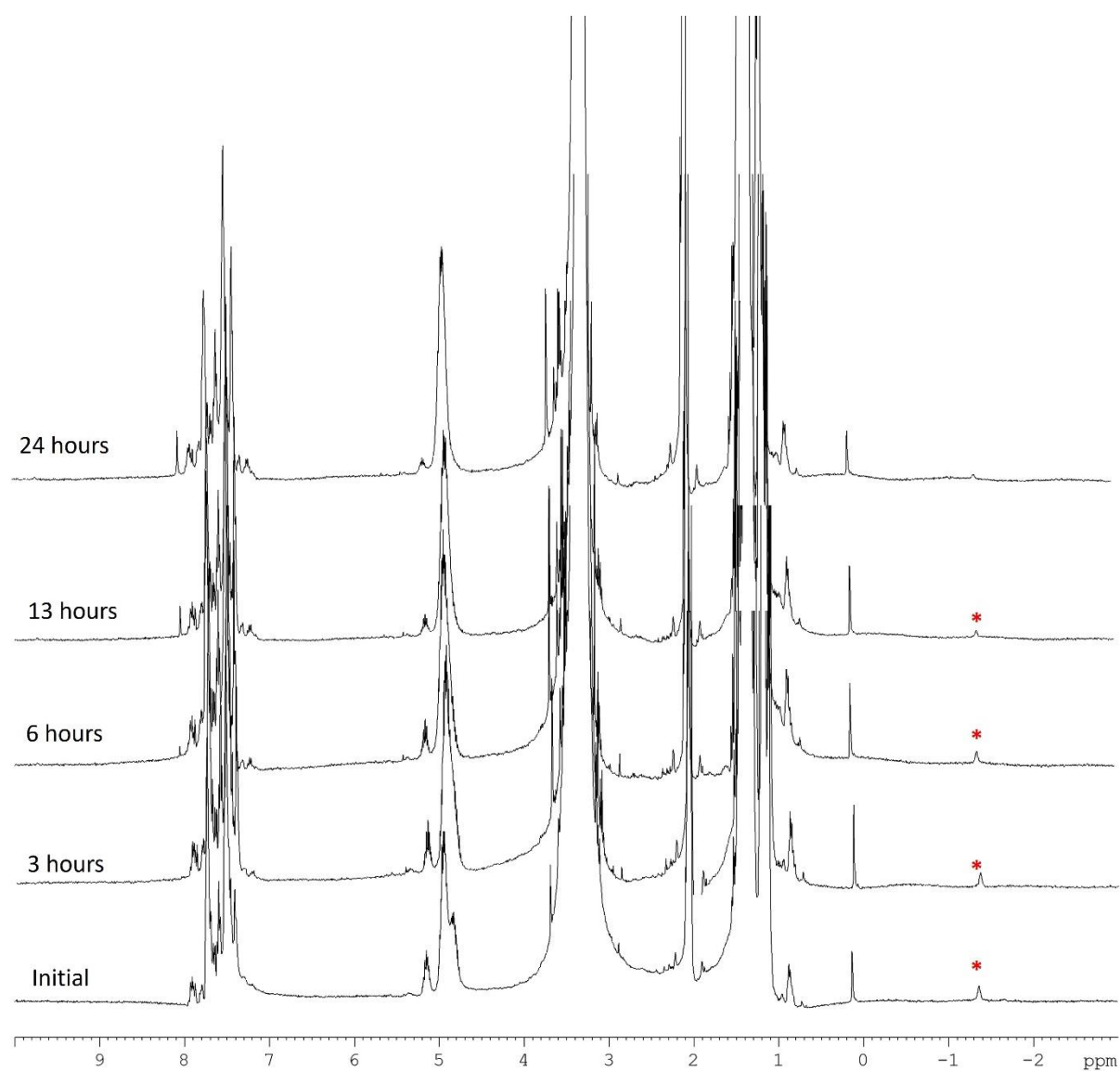


Figure S25. Structural transformation of **AuCu₁₁H** into **AuCu₁₂** in d_6 -acetone monitored by time-dependent ^1H NMR spectroscopy.

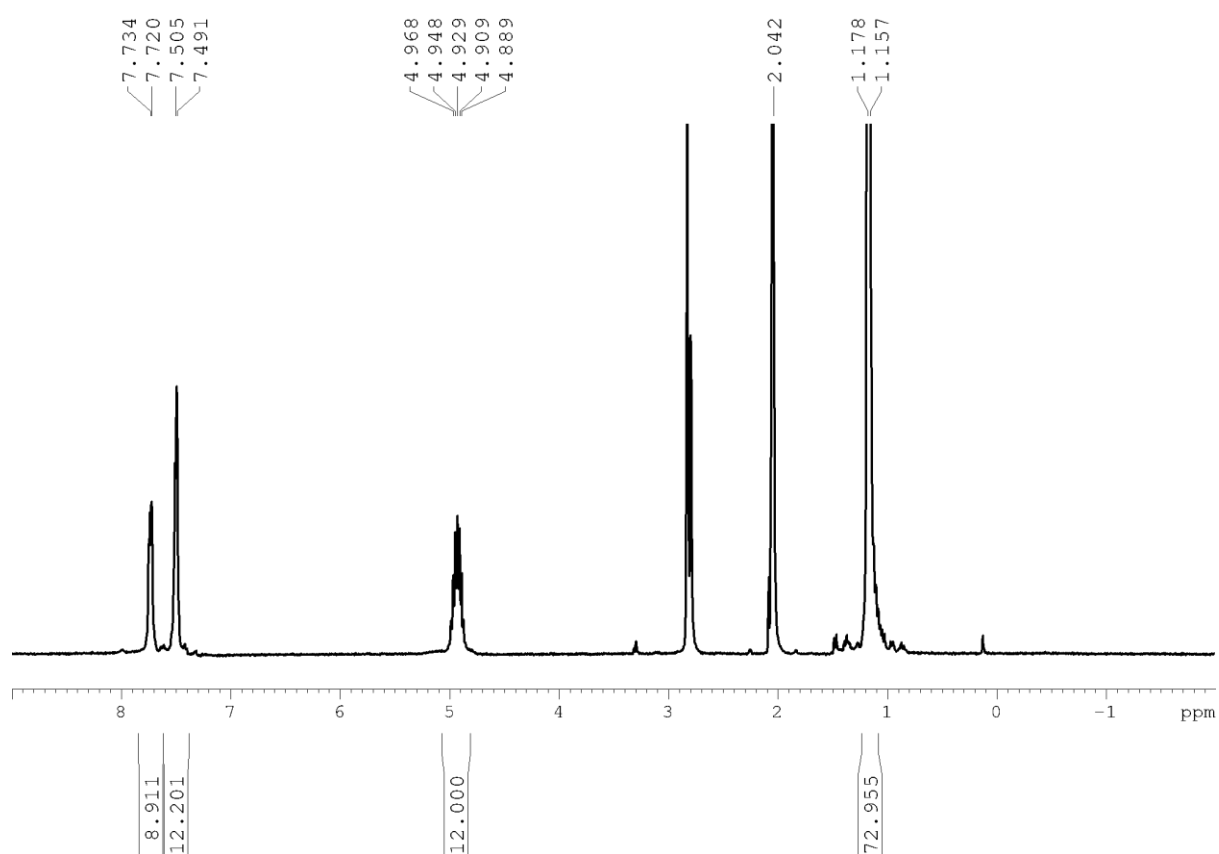


Figure S26. ^1H NMR spectrum of AuCu_{12} in d_6 -acetone.

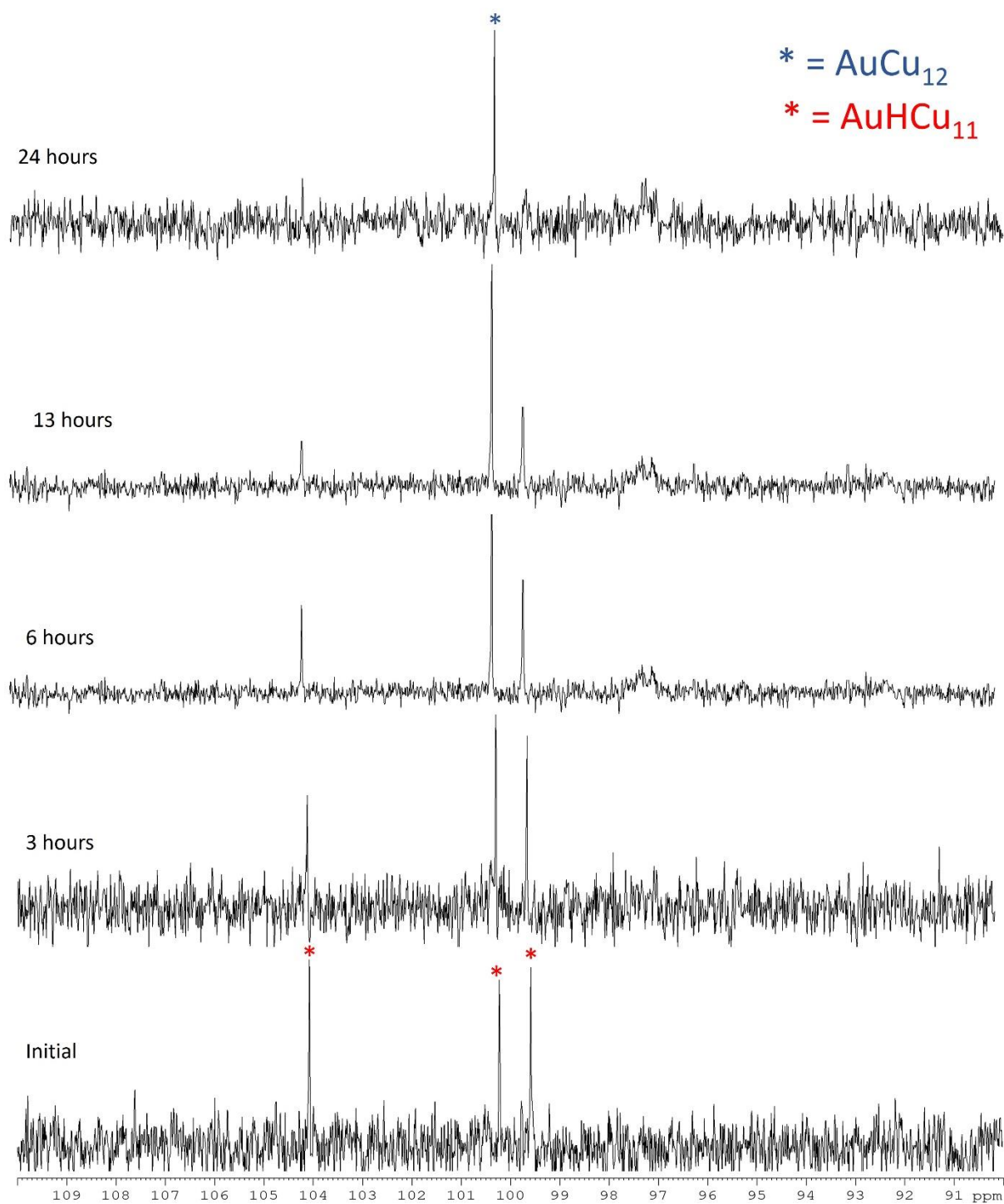


Figure S27. Structural transformation of AuCu_{11}H into AuCu_{12} in d_6 -acetone monitored by time-dependent $^{31}\text{P}\{^1\text{H}\}$ NMR spectroscopy.

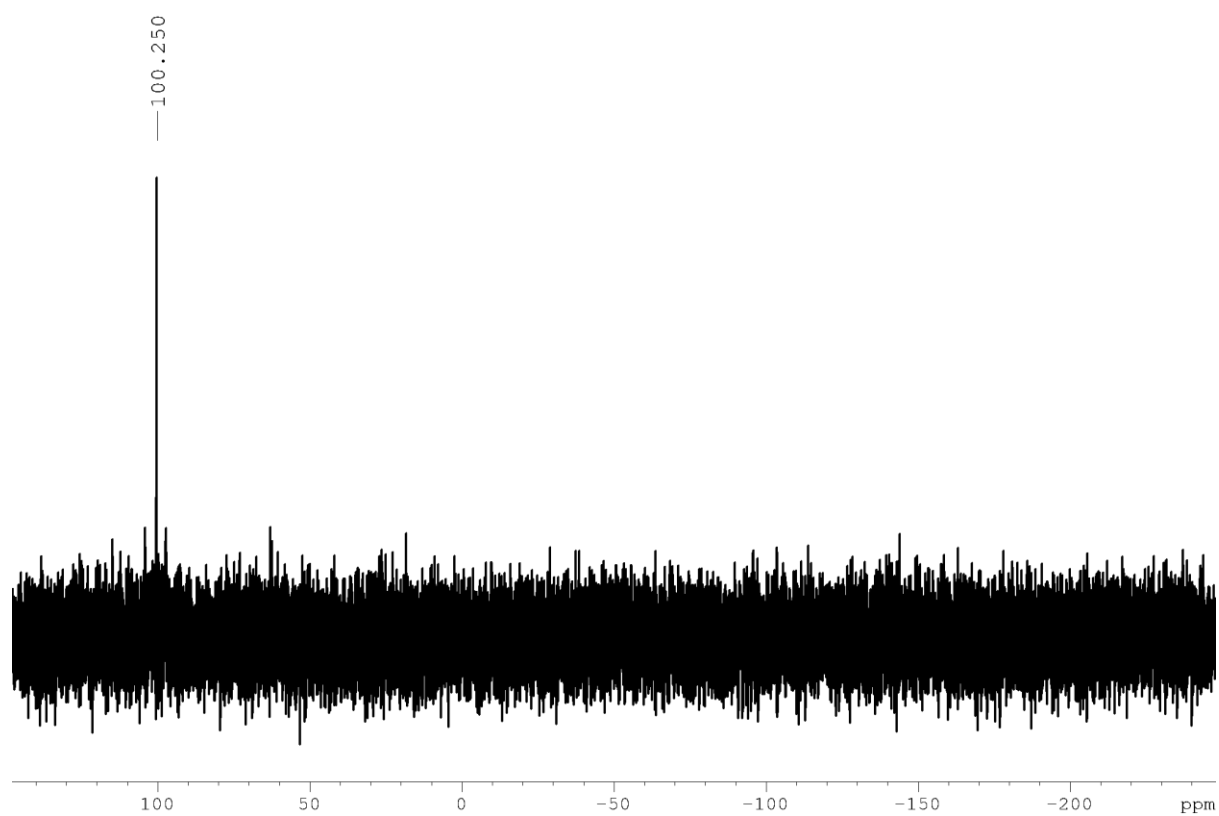


Figure S28. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **AuCu₁₂** in *d*₆-acetone.

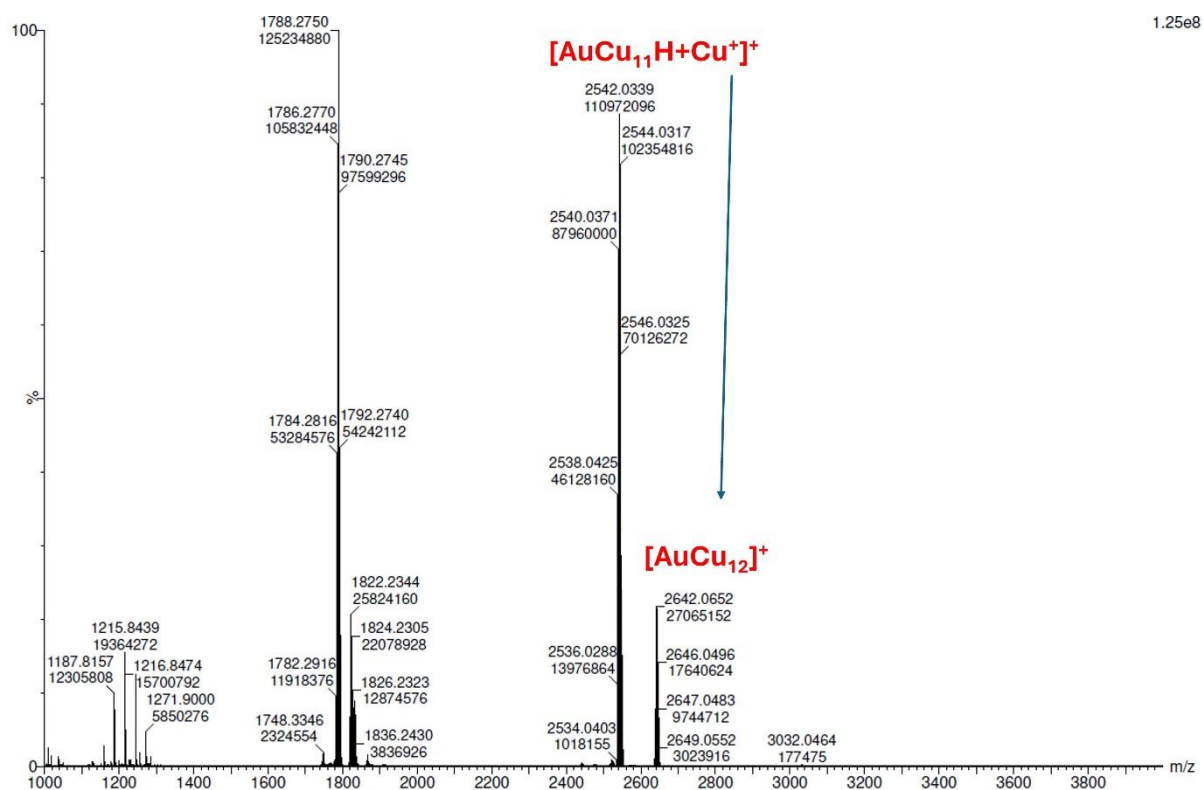


Figure S29. Positive-mode ESI-MS spectra of structural transformation of **AuCu₁₁H** in acetone.

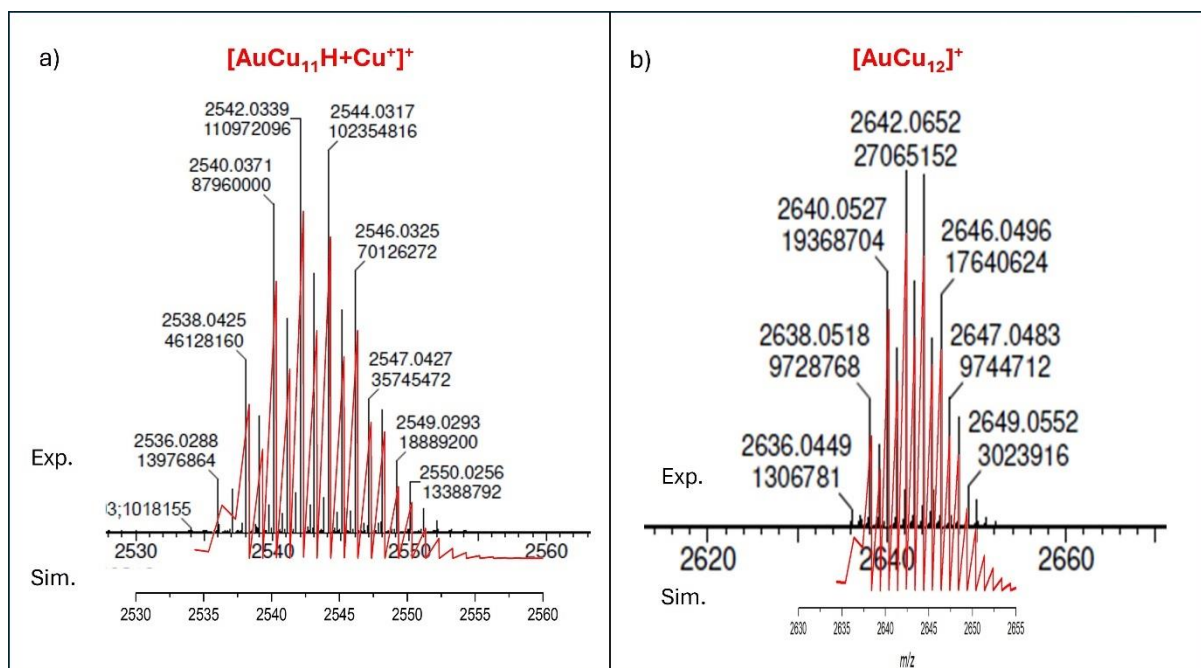


Figure S30. Isotope pattern of (a) AuCu_{11}H and (b) AuCu_{12} in structural transformation; inset show experimental (black) and simulated (red) isotopic distribution pattern.

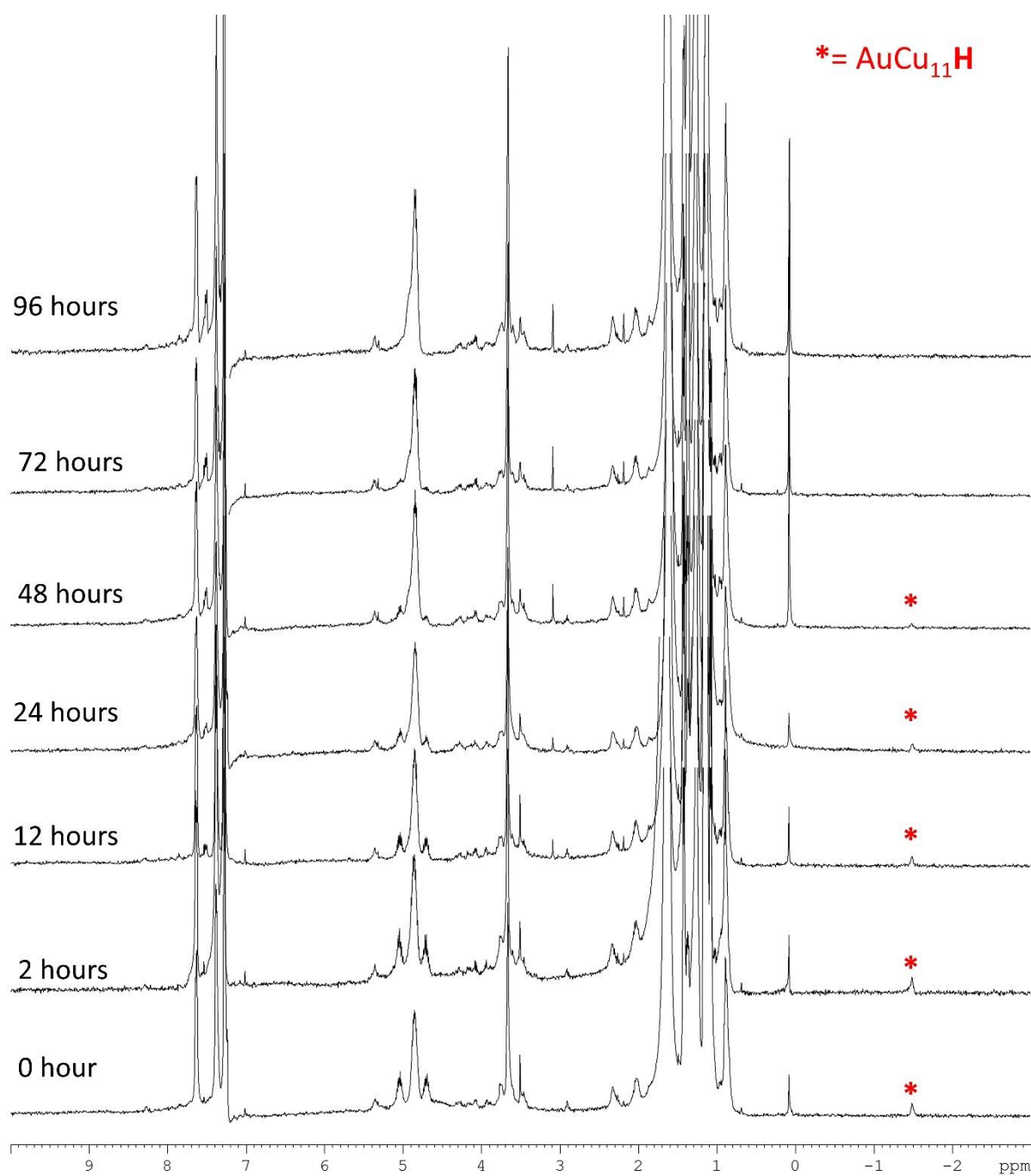


Figure S31. Structural transformation of AuCu_{11}H into AuCu_{12} via $\text{AuCu}_{11}\text{Cl}$ in CDCl_3 monitored by time-dependent ^1H NMR spectroscopy.

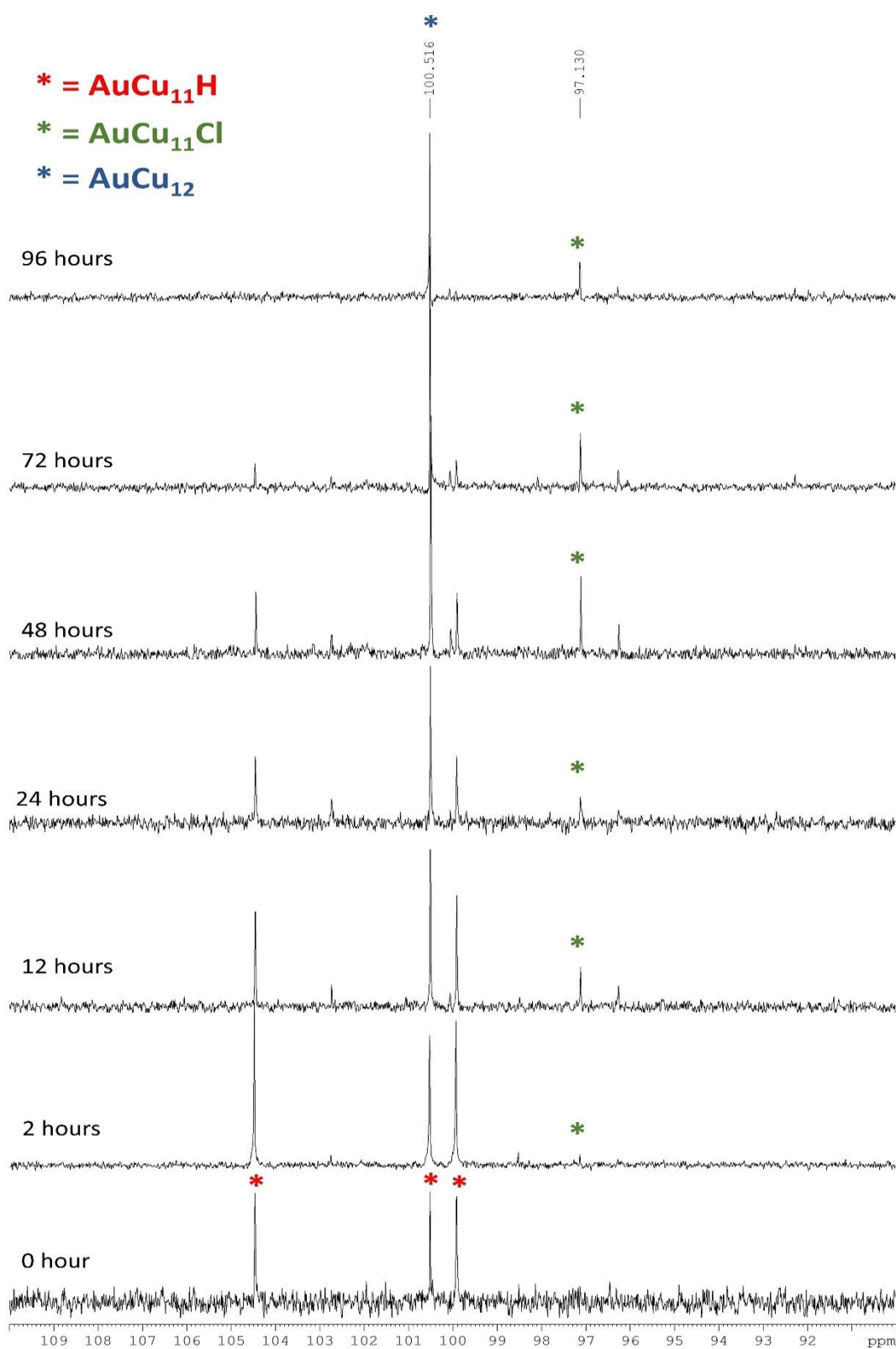


Figure S32. Structural transformation of AuCu_{11}H into AuCu_{12} via $\text{AuCu}_{11}\text{Cl}$ in CDCl_3 monitored by time-dependent $^{31}\text{P}\{^1\text{H}\}$ NMR spectroscopy.

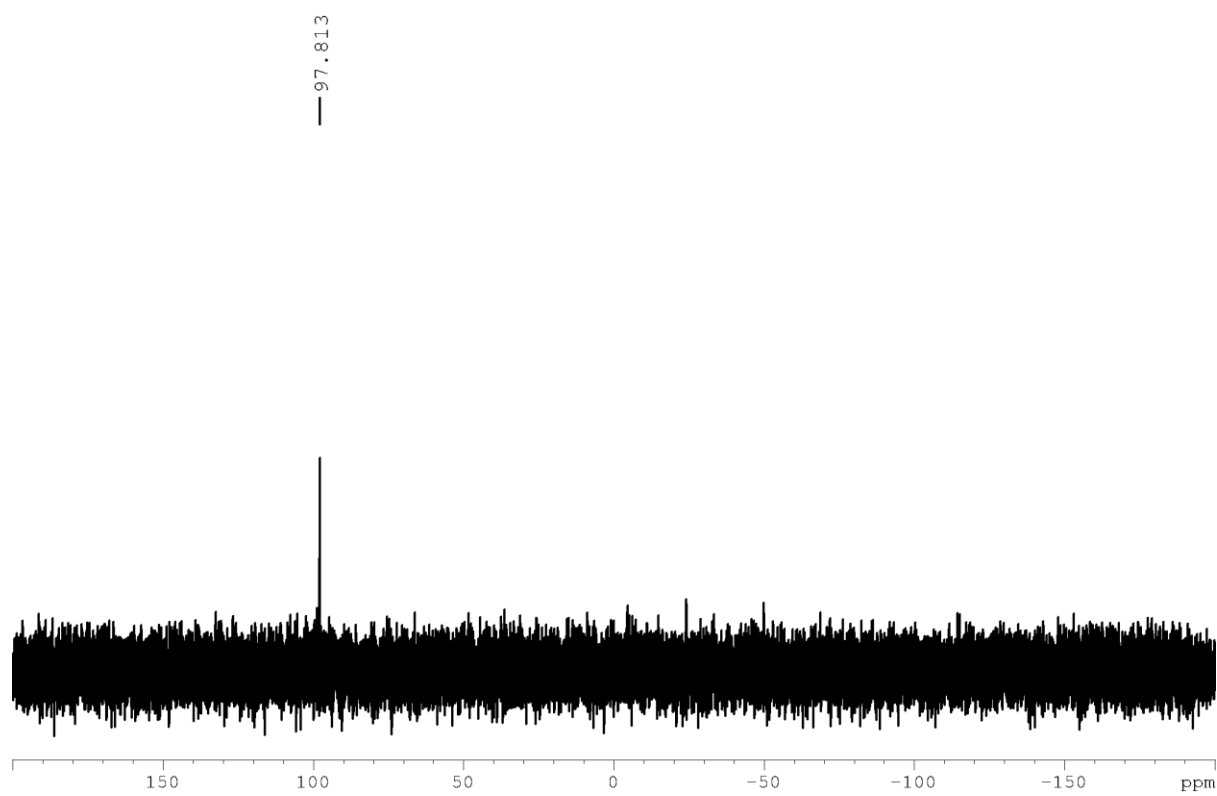


Figure S33. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **AuCu₁₁Cl** in CDCl_3 .

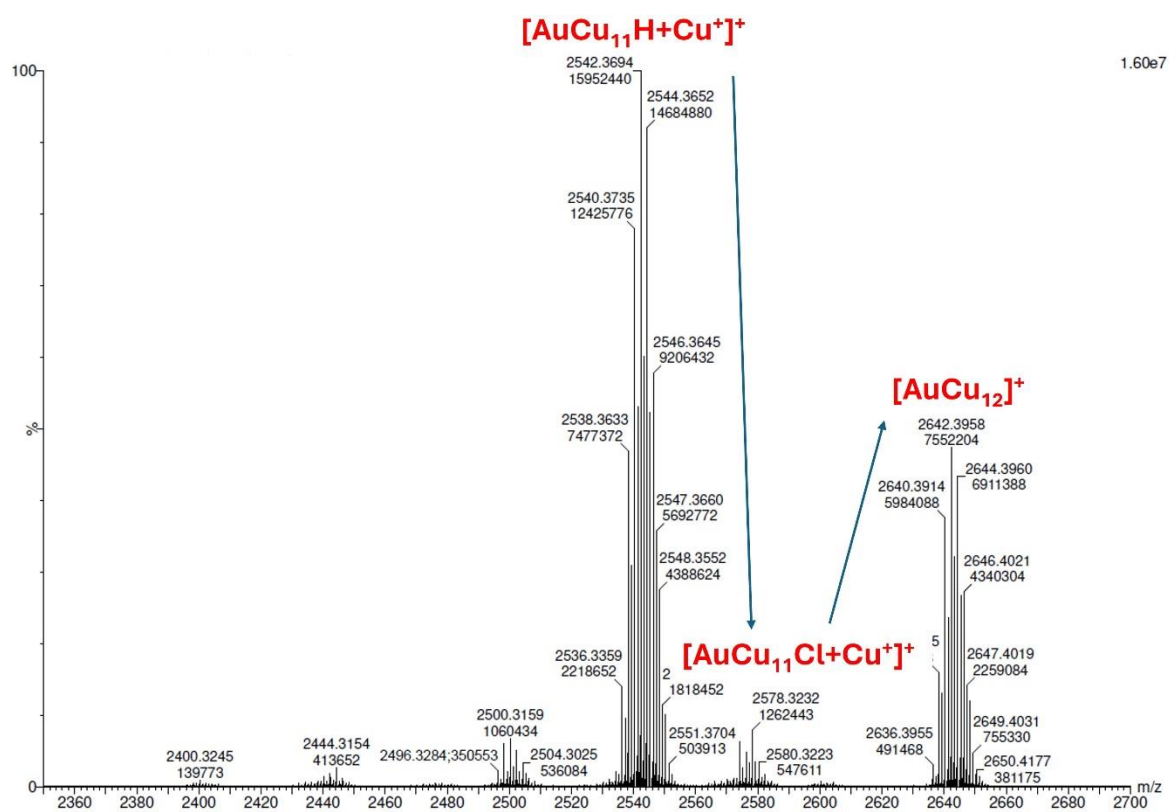


Figure S34. Positive-mode ESI-MS spectra of structural transformation of AuCu_{11}H in CH_2Cl_2 .

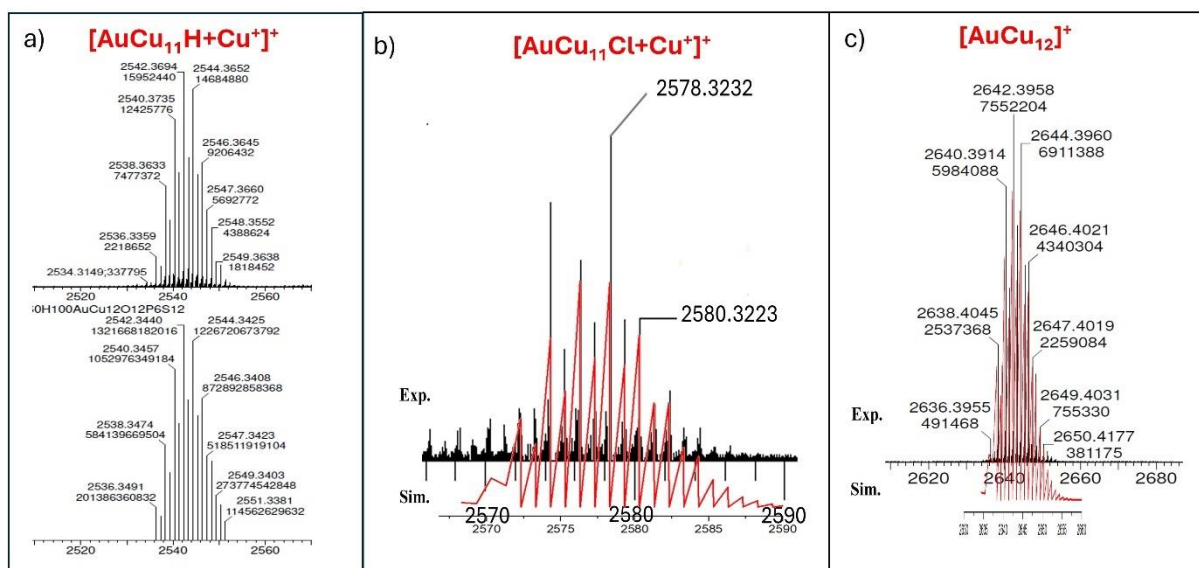


Figure S35. Isotope pattern of (a) AuCu_{11}H , (b) $\text{AuCu}_{11}\text{Cl}$, and (c) AuCu_{12} in structural transformation; inset show experimental (black) and simulated (red) isotopic distribution pattern.

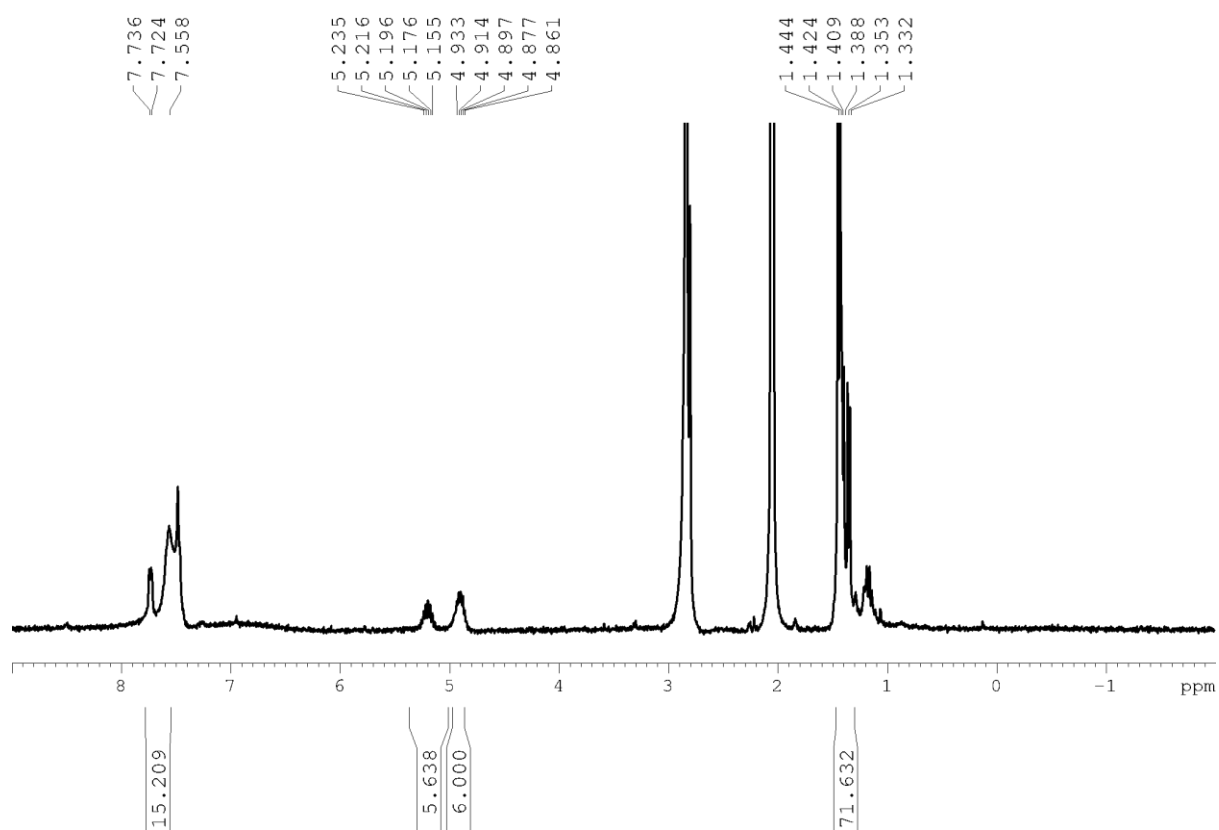
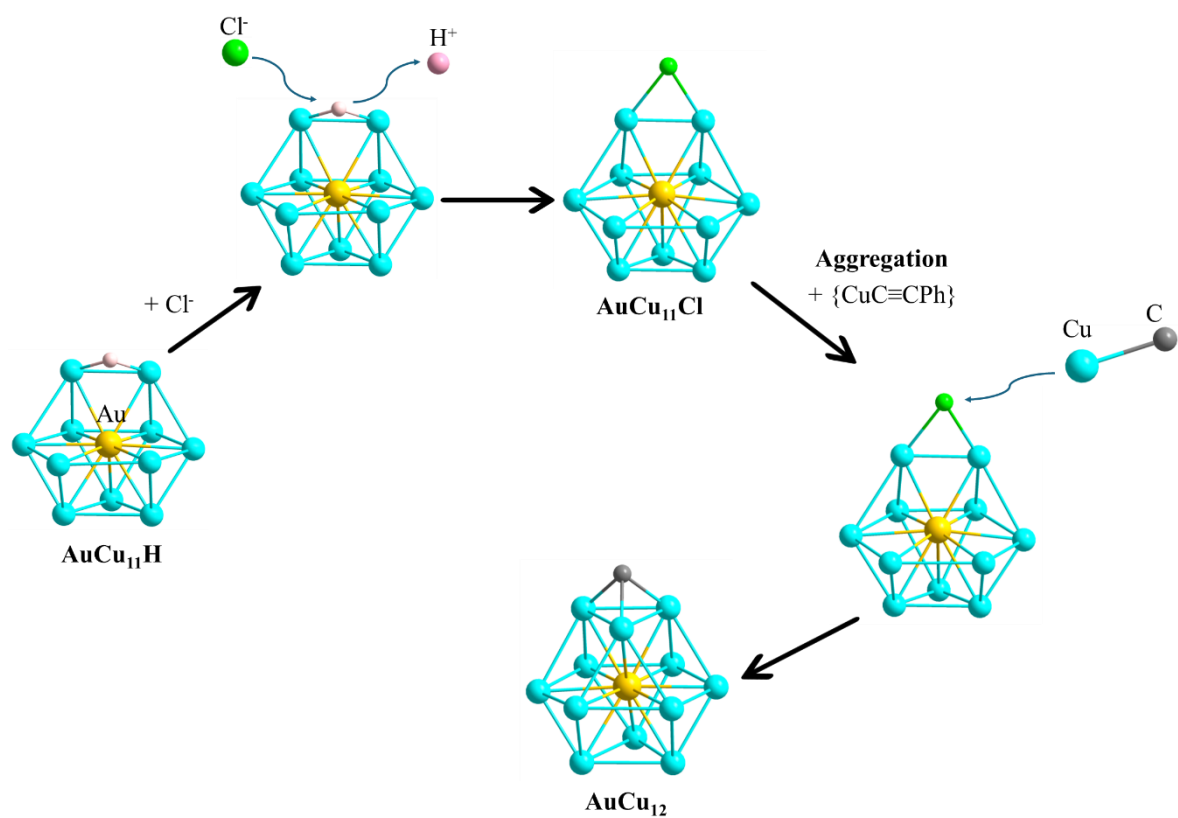


Figure S36. ¹H NMR spectrum of **AuCu₁₁Cl** in *d*₆-acetone.

Table S1. 298 K absorption, emission, and lifetime of **AuCu₁₁H**, **AuCu₁₁Cl**, and **AuCu₁₂**.

Compound	λ_{max} (nm)	λ_{em} (nm)	Lifetime, (μs)	Φ_{em}	k_{obs} , ^a $1/\tau(\mu\text{s}^{-1})$	k_{RAD} ^b (μs^{-1})	k_{NRD} ^c (μs^{-1})
AuCu₁₁H	318, 424, 487, 533	633	1.71	0.327	0.58	0.19	0.39
AuCu₁₁Cl	328, 432, 485, 540	606	3.75	0.033	0.27	0.009	0.26
AuCu₁₂	326, 433, 480, 540	637	3.20	0.32	0.31	0.10	0.21

^a $k_{\text{obs}} = k_{\text{RAD}} + k_{\text{NRD}}$, ^b $k_{\text{RAD}} = \Phi_{\text{em}}/\tau$, ^c $k_{\text{NRD}} = (1 - \Phi_{\text{em}})/\tau$; k_{RAD} = radiative rate constant, k_{obs} = mean excited-state decay rate constant, and k_{NRD} = nonradiative rate constant.



Scheme S1. A proposed mechanism of chloride-hydride ligand exchange, and aggregation within the transformation core of AuCu_{11}H to AuCu_{12} via $\text{AuCu}_{11}\text{Cl}$ in chloride-containing solvent.

Table S2. Cartesian coordinates of the DFT-optimezed structure of **AuCu₁₁H**.

Au	0.095621	-0.130302	0.333739
Cu1	-2.543087	-1.007363	0.601874
Cu2	-1.373752	-1.050237	-1.796426
Cu3	-0.704731	-2.861573	-0.048113
Cu4	-1.877508	1.860040	0.763614
Cu5	-0.673009	1.639173	-1.604270
Cu6	0.577234	2.669368	0.478096
Cu7	1.352161	-0.135480	-2.112966
Cu8	2.731650	0.705228	-0.097001
Cu9	2.169237	-1.969732	-0.259064
Cu10	1.422831	0.813534	2.540724
Cu11	-0.972821	-0.008806	2.850733
C1	3.203727	-0.655224	-1.521675
C2	4.204344	-1.309369	-1.823620
C3	5.352022	-2.072006	-2.159903
C4	5.537875	-3.342571	-1.600716
C5	6.656799	-4.089406	-1.924078
C6	7.608175	-3.589262	-2.803399
C7	7.434043	-2.329618	-3.361458
C8	6.317450	-1.576065	-3.045007
H1	4.798184	-3.724572	-0.907825
H2	6.787672	-5.071029	-1.482998
H3	8.483276	-4.178487	-3.052622
H4	8.173316	-1.932070	-4.047842
H5	6.179907	-0.593493	-3.479729
C9	-1.116415	3.324141	-0.410874
C10	-1.535832	4.253165	-1.101329
C11	-2.014162	5.294023	-1.936689
C12	-2.423111	6.524254	-1.406676
C13	-2.887854	7.528303	-2.238210
C14	-2.953105	7.325608	-3.610369
C15	-2.549029	6.109333	-4.145830

C16	-2.083341	5.099650	-3.322429
H6	-2.370129	6.681113	-0.336035
H7	-3.200645	8.475538	-1.813297
H8	-3.316543	8.113522	-4.260115
H9	-2.595937	5.945482	-5.216567
H10	-1.765827	4.149504	-3.734009
C17	-2.514336	-2.430249	-0.900338
C18	-3.509949	-3.154828	-0.913096
C19	-4.653059	-3.994055	-0.920026
C20	-4.517781	-5.385202	-0.828807
C21	-5.637557	-6.198546	-0.836898
C22	-6.907450	-5.644031	-0.927943
C23	-7.051916	-4.264821	-1.003651
C24	-5.938770	-3.442806	-0.999563
H11	-3.526880	-5.811978	-0.734005
H12	-5.518530	-7.273754	-0.763812
H13	-7.782071	-6.284355	-0.931433
H14	-8.041971	-3.826090	-1.060586
H15	-6.042837	-2.365205	-1.044948
S1	-3.962992	0.846689	0.241235
S2	-2.466600	0.782406	-2.893122
S3	0.127179	-1.558406	-3.568770
S4	1.105681	-3.850497	-1.190599
S5	-0.531826	-3.931276	1.996170
S6	-2.775695	-1.455175	2.871734
S7	-2.133591	2.037187	3.105004
S8	1.122077	3.147548	2.729016
S9	0.974202	1.927902	-3.295610
S10	2.691672	3.034428	-0.524038
S11	2.989242	-2.664259	1.790644
S12	3.684209	0.694761	2.042232
P1	-4.089862	1.051247	-1.752471
P2	0.896394	-3.371518	-3.127441
P3	-2.075059	-3.362462	3.074776

P4	-0.622656	3.188278	3.745478
P5	2.208758	3.269436	-2.471195
P6	4.277380	-1.250620	2.243106
O1	-5.249065	0.043490	-2.173441
O2	-4.600782	2.503969	-2.141220
O3	0.062208	-4.483768	-3.892996
O4	2.312691	-3.549955	-3.795048
O5	-3.294570	-4.344762	2.846087
O6	-1.797225	-3.596052	4.626347
O7	-0.398438	2.798195	5.257281
O8	-1.089961	4.701641	3.887366
O9	3.547692	3.391117	-3.317748
O10	1.576946	4.693313	-2.713539
O11	4.810966	-1.416117	3.737739
O12	5.624205	-1.441632	1.436276
C25	-5.666292	-0.108507	-3.558715
H16	-5.295723	0.755636	-4.120446
C26	-5.075787	-1.378063	-4.127667
H17	-3.987845	-1.360125	-4.072524
H18	-5.369869	-1.478894	-5.175431
H19	-5.440696	-2.249484	-3.580449
C27	-7.177949	-0.116718	-3.563839
H20	-7.584492	0.798502	-3.131116
H21	-7.554068	-0.966783	-2.990040
H22	-7.545321	-0.207063	-4.588499
C28	-5.799599	3.096376	-1.573565
H23	-6.398269	2.293699	-1.129340
C29	-5.410674	4.095766	-0.509140
H24	-4.835796	3.617707	0.283719
H25	-6.311910	4.531566	-0.070692
H26	-4.812207	4.898146	-0.944845
C30	-6.552031	3.734722	-2.718810
H27	-7.472721	4.192816	-2.350504
H28	-6.813561	3.001502	-3.483287

H29	-5.939691	4.512126	-3.181217
C31	-1.352500	-4.717531	-3.665524
H30	-1.685484	-4.062867	-2.854874
C32	-1.504378	-6.162999	-3.254652
H31	-1.119816	-6.823073	-4.036168
H32	-2.559558	-6.394757	-3.095080
H33	-0.958793	-6.361129	-2.330697
C33	-2.093781	-4.372333	-4.935452
H34	-1.755430	-5.004181	-5.760759
H35	-1.933607	-3.326791	-5.202809
H36	-3.164946	-4.532537	-4.793500
C34	2.489536	-3.423088	-5.234516
H37	1.515969	-3.191382	-5.677676
C35	2.982262	-4.755267	-5.747982
H38	3.933432	-5.013246	-5.276915
H39	3.133288	-4.705082	-6.828939
H40	2.259490	-5.543205	-5.532948
C36	3.445786	-2.284109	-5.490332
H41	3.059281	-1.356479	-5.066080
H42	3.577171	-2.148494	-6.566705
H43	4.419427	-2.495128	-5.043785
C37	-4.495229	-4.275586	3.661305
H44	-4.386326	-3.443184	4.363136
C38	-5.668057	-4.014942	2.747904
H45	-5.763389	-4.810973	2.006230
H46	-5.544507	-3.065737	2.225595
H47	-6.590295	-3.971658	3.332666
C39	-4.601294	-5.575171	4.425254
H48	-4.674936	-6.416859	3.732660
H49	-5.493677	-5.566796	5.055815
H50	-3.726598	-5.720531	5.060233
C40	-0.671938	-2.992120	5.309151
H51	-0.093235	-2.418538	4.577001
C41	-1.211052	-2.065668	6.374258

H52	-1.824801	-1.280980	5.929595
H53	-0.383934	-1.592800	6.909169
H54	-1.815943	-2.621537	7.095320
C42	0.173698	-4.116925	5.858851
H55	1.029625	-3.712845	6.403352
H56	0.544227	-4.747128	5.049278
H57	-0.412839	-4.732900	6.545334
C43	0.604785	3.442253	6.086063
H58	1.198065	4.107711	5.450639
C44	1.490488	2.353753	6.641915
H59	0.901085	1.654777	7.240187
H60	2.265835	2.788528	7.276946
H61	1.971127	1.803188	5.832454
C45	-0.111917	4.243635	7.147363
H62	-0.750531	5.001767	6.692924
H63	0.615588	4.740986	7.793167
H64	-0.731305	3.588641	7.764327
C46	-1.446159	5.507108	2.734399
H65	-1.328072	4.895744	1.833774
C47	-0.496474	6.680668	2.680735
H66	-0.730839	7.314576	1.822277
H67	0.534221	6.336772	2.582401
H68	-0.582251	7.284002	3.588023
C48	-2.894767	5.906316	2.893545
H69	-3.032134	6.487563	3.808674
H70	-3.533521	5.023272	2.940269
H71	-3.213082	6.518175	2.046317
C49	4.503954	2.306540	-3.434608
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C51	5.814068	2.783841	-2.853546

H76	6.180942	3.655432	-3.401596
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H80	3.122261	6.099012	-4.336697
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H82	1.577897	6.940797	-4.100240
C54	1.472760	6.656817	-1.337057
H83	0.506566	6.941619	-1.758217
H84	2.001193	7.563261	-1.031604
H85	1.301738	6.038626	-0.454716
C55	3.939992	-1.307849	4.885569
H86	2.930282	-1.069840	4.531852
C56	3.932990	-2.647186	5.585317
H87	4.945880	-2.919495	5.892264
H88	3.545905	-3.423620	4.924370
H89	3.304694	-2.600837	6.477930
C57	4.459844	-0.183054	5.751033
H90	5.481153	-0.396256	6.076734
H91	3.832510	-0.069266	6.638108
H92	4.457680	0.758724	5.199926
C58	6.790371	-0.612877	1.683708
H93	6.527592	0.131098	2.442083
C59	7.149185	0.086719	0.394791
H94	8.015939	0.733276	0.553086
H95	6.315758	0.699571	0.048472
H96	7.394557	-0.641806	-0.380796
C60	7.886659	-1.511859	2.206693
H97	7.575955	-1.999146	3.131599
H98	8.787728	-0.926422	2.405296
H99	8.128676	-2.280757	1.469327
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Cu	-0.968069	-1.736219	-1.885585
Cu	0.417774	-2.845302	-0.045194
Cu	-2.373123	1.234931	0.734250
Cu	-1.366626	1.458992	-1.662982
Cu	-0.460255	2.693157	0.379616
Cu	1.409896	0.366213	-2.264067
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Cu	2.683178	-1.307658	-0.185118
Cu	0.957193	1.609882	2.134186
Cu	-1.221887	-0.136210	2.543186
C	3.206272	0.370117	-1.416823
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C	6.106283	-1.820934	-1.366272
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C	8.172040	-1.536271	-2.568182
C	7.685379	-0.361488	-3.127295
C	6.414817	0.084376	-2.810910
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C	-1.412808	-3.340212	-0.777699
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S	2.484718	-3.507206	-1.315251
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P	-4.153648	-0.501622	-1.589030
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C	-5.266718	-2.215568	-3.305432
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C	0.698204	-6.382159	-3.239176
H	1.223821	-6.895796	-4.048134
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H	1.348537	-6.345814	-2.364229
C	-0.599767	-4.960785	-4.876382
H	-0.117469	-5.451459	-5.725712
H	-0.839836	-3.933495	-5.155170
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C	3.399527	-2.416242	-5.371342
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C	4.022196	-1.056876	-5.577723
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H	5.042482	-1.043074	-5.188543
C	-2.537658	-5.275814	4.319948
H	-2.585733	-4.332328	4.871930
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H	1.377775	-1.235828	6.328240
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C	2.286417	-3.727255	5.439720
H	3.119783	-3.079749	5.718198
H	2.613863	-4.383530	4.632585
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C	-0.706225	3.753647	6.081016
H	-0.413032	4.585109	5.432163
C	0.530256	3.073938	6.618334
H	0.253849	2.206023	7.221891
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C	-1.646247	4.243739	7.157219
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H	3.387309	-0.088322	4.613522
C	5.088056	-0.847953	5.675370
H	6.104358	-0.539003	5.931886
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C	4.306400	1.552472	5.651379
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C	6.561434	1.852588	1.497216
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H	7.120652	3.506256	0.252347
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C	7.944753	1.462965	1.964459
H	7.894522	0.939274	2.919770
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