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Supporting information for article:

Crystal structure of bulky-ligand-protected $Au_{24}(S\text{-}C_4H_9)_{16}$

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Computing details

For the $Au_{24}(S\text{-}t\text{Bu})_{16}$ structure, data collection: *APEX3* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2019); data reduction: *SAINT* (Bruker, 2019); programs used to solve structure: *ShelXT* (Sheldrick, 2015a); programs used to refine structure: *ShelXL* (Sheldrick, 2015b); molecular graphics; *CrystalMaker* (Palmer, 2014)

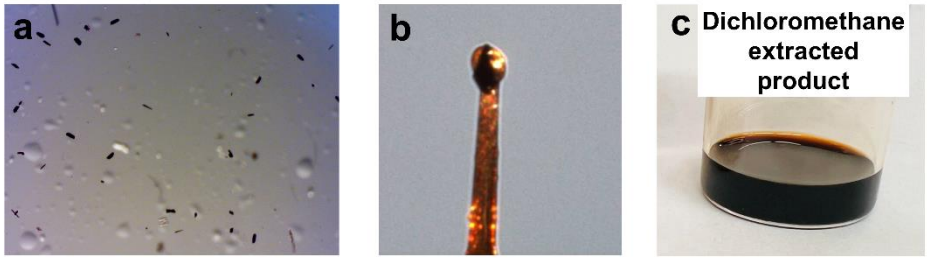

Figure S1. Images of the (a) $Au_{24}(S\text{-}t\text{Bu})_{16}$ crystal under the light microscope (b) $Au_{24}(S\text{-}t\text{Bu})_{16}$ crystal in the sc-xray diffractometer and (c) dichloromethane extracted product.

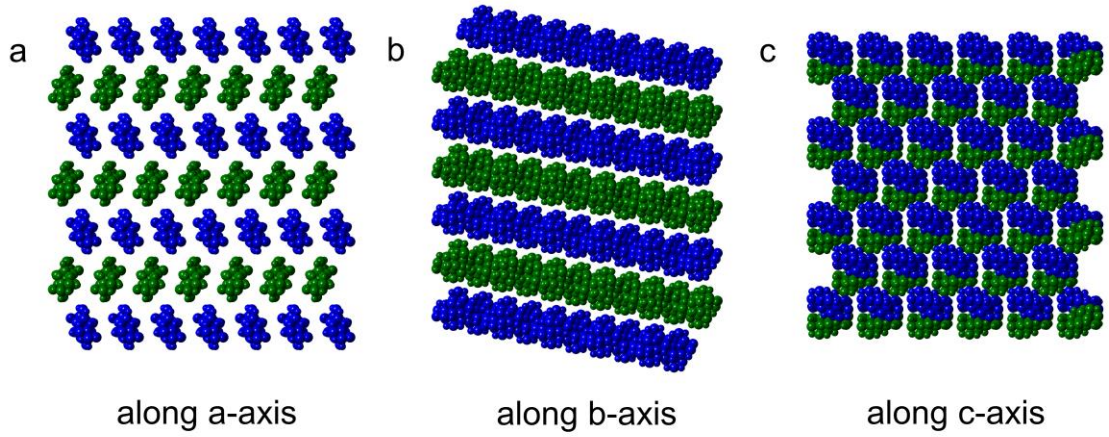

Figure S2 Packing structures are viewed along the (a) a-axis (b) b-axis and (c) c-axis. Blue and Green; Au, Yellow; S, Black; C, Pink; H. Carbon and H atoms were omitted for clarity.

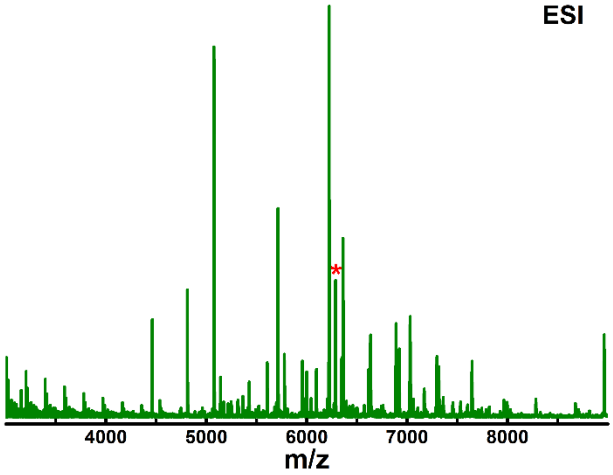

Figure S3 ESI-MS for the DCM soluble portion of the crude. The * indicates the $Au_{24}(S\text{-}t\text{Bu})_{16}$

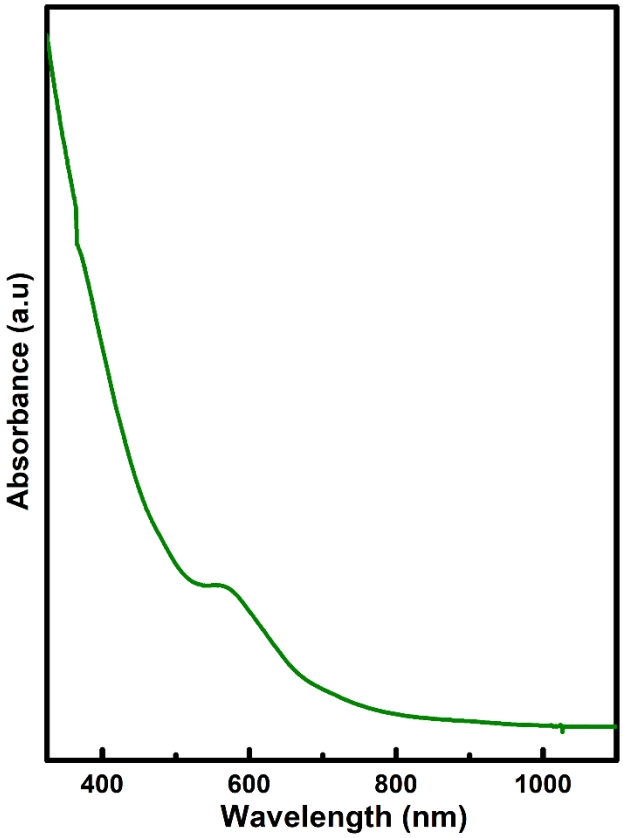

Figure S4 UV-visible spectra of $Au_{24}(S\text{-}t\text{Bu})_{16}$ crude in toluene

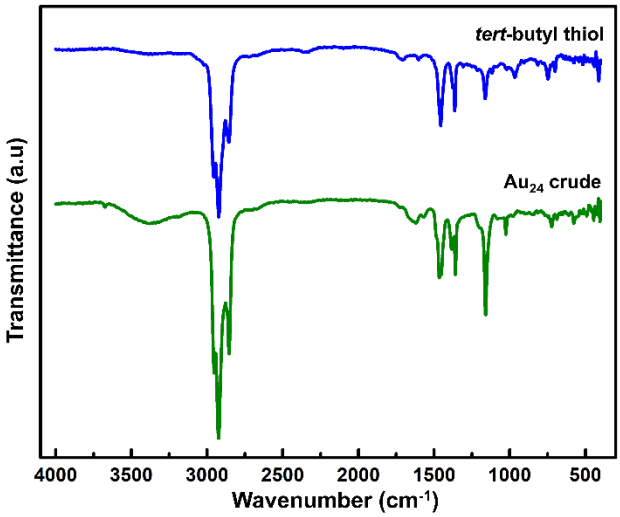

Figure S5 IR spectra of the *tert*-butyl thiol (top) and $Au_{24}(S\text{-}tBu)_{16}$ crude (bottom)

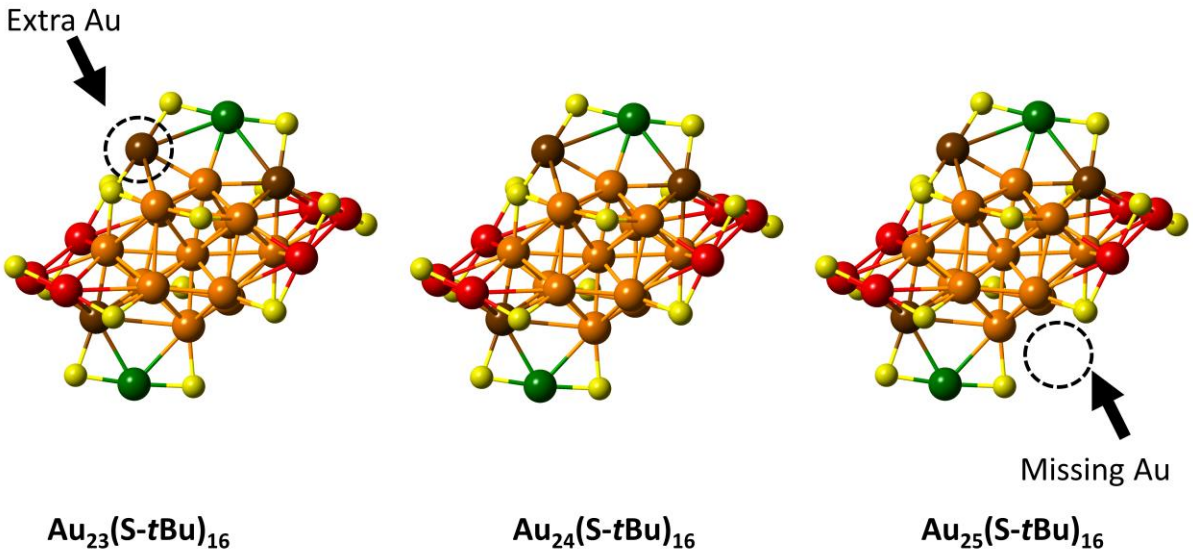

Figure S6 Predicted crystal structure of $Au_{23}(S\text{-}tBu)_{16}$ and $Au_{25}(S\text{-}tBu)_{16}$ based on the $Au_{24}(S\text{-}tBu)_{16}$ structure. Core Au: orange, capping Au: brown, monomeric Au: green, trimeric Au: red, and S: yellow.

Table S1. Selected AuNM crystal structures protected by various thiol ligands

Composition	**Ligand**	**Core**	**Staples**	**Ref.**
Au_{21}(S-Adm)$_{15}$	1-adamantanethiol	Two octahedrons sharing one edge to form Au_{10} kernel	[RS-Au-SR] [RS-Au-SR-Au-SR] $Au_8(SR)_9$ motif bridging [SR]	(Chen *et al.*, 2016)
Au_{21}(S-*t*Bu)$_{15}$	*tert*-butyl thiol	Au_{10} kernel	2[RS-Au-SR-Au-SR] [RS-Au-SR-Au-SR-Au-SR] $Au_4(SR)_5$ motif	(Xiong *et al.*, 2018)
$Au_{23}(SC_6H_{11})_{16}$	cyclohexanethiol	Au_{15} cuboctahedral based bipyramidal structure	2[RS-Au-SR] 2[RS-Au-SR-Au-SR-Au-SR] 4 bridging [SR]	(Das *et al.*, 2013)
$Au_{24}(SCH_2Ph\text{-}tBu)_{20}$	4-*tert*-butylbenzylmercaptan	Bitetrahedral Au_8 kernel	4[$Au_4(SR)_5$ motif]	(Das *et al.*, 2014)
$Au_{24}(PPh_3)_{10}(SC_2H_4Ph)_5X_2$	Triphenylphosphine and Phenylethyl thiol	Au_{24} core (two incomplete Au_{12} icosahedral units)	-	(Das *et al.*, 2012)
Au_{24}(SAdm)$_{16}$	1-adamantanethiol	Au_{13} cuboctahedra + 2Au atoms capped onto two 100 square faces	2[RS-Au-SR] 2[RS-Au-SR-Au-SR-Au-SR]	(Crasto, Barcaro, *et al.*, 2014)
$Au_{25}(SCH_2CH_2Ph)_{18}$	Phenylethyl thiol	Au_{13} icosahedra	6[RS-Au-SR-Au-SR]	(Heaven *et al.*, 2008)

Au_{30}(S-Adm)$_{18}$	1-adamantanethiol	Au_{18} kernel	6[RS-Au-SR-Au-SR]	(Higaki *et al.*, 2016)
Au_{30}(S-*t*Bu)$_{18}$	*tert*-butyl thiol	Au_{20} interpenetrating bicuboctahedra	2[RS-Au-SR] 2[RS-Au-SR-Au-SR-Au-SR] 4 bridging [SR]	(Dass *et al.*, 2016)
$Au_{144}(SCH_2Ph)_{60}$	benzyl mercaptan	Au_{12} + Au_{42} + Au_{60}	30[RS-Au-SR]	(Yan *et al.*, 2018)
Au_{133}(SPh-*t*Bu)$_{52}$	4-*tert*-butylbenzene thiol	Au_{13} + Au_{42} + Au_{52}	26[RS-Au-SR]	(Dass *et al.*, 2015)
Au_{191}(SPh-*t*Bu)$_{66}$	4-*tert*-butylbenzene thiol	Au_{26} + Au_{63} + Au_{66}	24[RS-Au-SR] 6[RS-Au-SR-Au-SR]	(Sakthivel *et al.*, 2020)
Au_{279}(SPh-*t*Bu)$_{84}$	4-*tert*-butylbenzene thiol	Au_{13} + Au_{42} + Au_{92} + Au_{102}	18[RS-Au-SR] 6[RS-Au-SR-Au-SR] 30 bridging [SR]	(Sakthivel *et al.*, 2017)

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 20210518_008_Au24_bruker. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Au1	4865.6(7)	3940.8(4)	4837.5(3)	27.0(2)
Au2	6370.2(7)	3535.8(4)	5473.1(3)	30.0(2)
Au3	6808.7(7)	4451.5(4)	5151.2(3)	28.8(2)
Au4	3467.5(7)	4426.5(4)	5123.3(3)	29.5(2)
Au5	6269.9(7)	3519.7(4)	4485.6(3)	30.3(2)
Au6	4690.6(7)	3887.7(4)	5736.8(3)	31.6(2)
Au7	5144.9(7)	4786.9(4)	5371.2(4)	32.2(2)
Au8	4826.7(7)	3967.0(4)	3917.0(3)	31.7(2)
Au9	3351.9(7)	4416.3(4)	4135.3(3)	30.6(2)
Au10	4471.9(7)	2886.2(4)	5284.2(4)	32.4(2)
Au11	1587.1(7)	4363.6(4)	4333.5(4)	33.7(2)
Au12	3005.8(7)	3469.8(4)	4442.1(4)	30.9(2)
Au13	4678.2(7)	3046.3(4)	4327.2(4)	33.5(2)
Au14	5226.3(7)	5026.6(4)	4340.8(4)	31.8(2)
Au15	6904.3(7)	4325.4(4)	6038.3(3)	32.8(2)
Au16	3154.7(8)	3575.3(4)	3577.0(4)	33.7(2)
Au17	6468.6(7)	4272.4(4)	3763.1(3)	33.4(2)
Au18	8622.3(8)	4583.0(5)	5845.5(4)	36.6(2)
Au19	1345.4(8)	3377.8(4)	3654.1(4)	36.6(2)
Au20	6986.4(8)	5445.4(4)	5774.7(4)	37.0(2)
Au21	8208.4(8)	3595.3(4)	5201.0(4)	36.1(2)
Au22	4777.7(8)	3629.8(5)	3010.4(4)	39.5(3)
Au23	5768.5(8)	4059.9(5)	6696.3(4)	38.8(3)
Au24	2895.7(8)	2442.7(5)	3792.7(5)	43.5(3)
S1	3792(5)	5289(2)	4255(2)	33.7(13)
S2	1957(4)	4502(3)	5107(2)	33.9(13)
S3	3025(4)	3149(3)	5186(2)	33.2(13)
S4	6676(4)	4812(2)	4396.4(19)	29.6(12)
S5	5930(5)	2664(2)	5378(2)	35.1(13)
S6	6245(5)	3808(3)	3095(2)	40.2(15)

Atom	***x***	***y***	***z***	**U(eq)**
S7	1151(5)	4257(3)	3547(2)	36.2(13)
S8	4457(5)	3652(3)	6472(2)	37.1(14)
S9	1405(5)	2500(3)	3749(3)	41.1(15)
S10	8451(5)	5459(3)	5722(3)	39.7(14)
S11	5559(5)	5487(3)	5873(2)	37.7(14)
S12	7770(5)	3453(3)	4424(2)	35.5(13)
S13	3348(5)	3370(3)	2826(2)	42.1(15)
S14	8808(4)	3707(3)	5964(2)	37.4(14)
S15	4378(5)	2355(3)	3802(3)	44.1(16)
S16	7079(5)	4483(3)	6837(2)	43.5(16)
C1	7140(20)	5830(11)	4569(11)	43(7)
C2	7400(20)	5351(10)	4308(9)	35(6)
C3	3810(20)	4676(15)	6533(14)	62(10)
C4	1960(20)	5293(12)	5693(9)	39(6)
C5	5340(30)	6255(14)	5205(18)	73(12)
C6	7840(20)	4058(12)	7189(9)	42(7)
C7	8310(20)	5198(10)	4463(10)	37(6)
C8	7319(19)	2423(14)	6061(12)	47(7)
C9	6300(20)	2336(11)	5943(11)	43(7)
C10	8850(30)	6357(13)	6167(13)	55(9)
C11	5110(20)	6119(14)	5644(16)	56(9)
C12	5450(30)	6507(12)	5982(13)	65(11)
C13	1960(30)	5538(12)	4877(12)	53(9)
C14	-50(20)	4377(14)	3395(13)	52(8)
C15	10050(20)	2977(15)	5986(17)	66(11)
C16	10024(18)	3563(13)	6042(10)	41(7)
C17	3110(30)	3840(20)	1982(11)	76(14)
C18	2390(20)	2521(10)	5738(11)	41(7)
C19	7590(30)	4060(20)	7669(12)	72(13)
C20	1630(20)	5183(12)	5190(11)	44(7)
C21	3810(30)	6205(16)	3830(19)	81(15)
C22	7790(20)	2413(13)	4659(10)	47(8)
C23	3670(20)	4053(18)	7162(12)	65(12)

Atom	*x*	*y*	*z*	U(eq)
C24	3655(16)	4095(13)	6628(11)	41(7)
C25	950(30)	1609(14)	3230(20)	80(15)
C26	1260(30)	2370(15)	2814(13)	72(13)
C27	8790(20)	4253(18)	7218(12)	60(10)
C28	1390(20)	2740(12)	5030(13)	48(8)
C29	2770(30)	3848(17)	2415(11)	61(10)
C30	6110(30)	1772(16)	5872(15)	68(12)
C31	6030(20)	3995(19)	2164(11)	64(11)
C32	2910(30)	4405(12)	2617(14)	63(10)
C34	5780(20)	4771(15)	2653(14)	57(9)
C33	7760(20)	3491(12)	7014(13)	51(8)
C35	5870(30)	2576(19)	6311(12)	71(13)
C36	7250(20)	4418(15)	2671(12)	56(10)
C37	850(30)	2187(14)	3188(17)	66(11)
C38	-150(30)	4979(14)	3481(13)	59(9)
C39	4750(20)	1750(15)	4063(15)	58(9)
C40	8040(20)	2775(11)	4319(10)	40(6)
C41	2760(30)	3929(17)	6382(12)	63(10)
C42	9950(30)	5679(17)	6287(17)	77(15)
C43	5770(30)	1743(17)	4170(20)	87(15)
C44	7590(30)	2641(14)	3862(12)	56(9)
C45	2600(30)	2104(12)	5022(14)	56(9)
C46	660(20)	5193(13)	5101(10)	45(7)
C47	9050(30)	2756(16)	4348(16)	69(11)
C48	4440(30)	1320(11)	3707(14)	57(9)
C49	8720(30)	5597(17)	6665(10)	61(11)
C50	10410(30)	3818(14)	5685(14)	58(9)
C51	6290(20)	4284(12)	2611(10)	42(7)
C52	-272(19)	4280(16)	2880(11)	54(10)
C53	2300(20)	2578(11)	5242(10)	38(7)
C54	10400(30)	3730(19)	6535(11)	71(13)
C55	-60(20)	2320(20)	3155(18)	83(15)
C56	-550(20)	4075(17)	3673(13)	60(11)

Atom	***x***	***y***	***z***	**U(eq)**
C57	9040(30)	5784(16)	6253(14)	61(10)
C58	1880(30)	3680(20)	2335(13)	81(15)
C59	2530(30)	5628(18)	3560(16)	71(11)
C60	4370(20)	1631(14)	4508(12)	53(8)
C61	3580(20)	5663(13)	3712(13)	52(9)
C62	4040(30)	6050(20)	5590(20)	86(15)
C63	3850(60)	5420(20)	3365(15)	150(40)
C64	7220(20)	5497(10)	3794(8)	34(6)

Table 1 **Table S3.** Anisotropic Displacement Parameters ($Å^2×10^3$) for 20210518_008_Au24_bruker. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Au1	31.1(5)	27.0(4)	21.7(4)	-0.5(3)	1.5(4)	3.9(4)
Au2	34.7(5)	29.5(5)	24.0(5)	3.0(4)	1.1(4)	2.9(4)
Au3	34.5(5)	28.5(5)	23.0(5)	1.8(4)	3.9(4)	2.4(4)
Au4	31.4(5)	30.8(5)	25.0(5)	1.5(4)	2.2(4)	5.0(4)
Au5	32.9(5)	32.0(5)	25.1(5)	1.8(4)	2.8(4)	4.5(4)
Au6	38.4(6)	32.3(5)	22.9(5)	1.7(4)	2.3(4)	4.2(4)
Au7	35.8(6)	30.0(5)	30.1(5)	-4.3(4)	4.4(4)	0.3(4)
Au8	34.8(5)	36.7(5)	21.9(5)	1.2(4)	0.7(4)	4.1(4)
Au9	34.2(5)	29.5(5)	26.8(5)	2.1(4)	2.3(4)	3.0(4)
Au10	36.8(6)	28.9(5)	30.5(5)	1.6(4)	3.3(4)	0.6(4)
Au11	34.1(6)	34.4(5)	30.8(5)	-1.6(4)	1.1(4)	3.2(5)
Au12	34.4(5)	29.5(5)	27.8(5)	2.0(4)	2.8(4)	3.3(4)
Au13	37.8(6)	28.4(5)	32.8(5)	-4.1(4)	2.7(4)	1.5(4)
Au14	35.3(5)	31.2(5)	27.8(5)	1.5(4)	3.3(4)	0.8(4)
Au15	38.5(6)	37.4(5)	22.0(5)	-0.8(4)	4.5(4)	0.9(5)
Au16	35.9(6)	38.1(5)	25.0(5)	-2.7(4)	-0.1(4)	1.0(5)
Au17	38.3(6)	38.4(5)	22.7(5)	1.4(4)	3.4(4)	1.4(5)
Au18	37.3(6)	37.9(6)	34.0(5)	-1.9(4)	4.9(4)	3.2(5)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au19	36.7(6)	32.9(5)	38.3(6)	-3.1(4)	2.4(5)	3.9(5)
Au20	39.3(6)	33.3(5)	36.6(6)	-3.4(4)	2.0(5)	2.4(5)
Au21	35.7(6)	35.0(5)	36.7(6)	-0.6(4)	4.4(5)	3.2(5)
Au22	46.9(7)	45.5(6)	25.7(5)	-3.9(4)	5.3(5)	-2.7(5)
Au23	38.3(6)	51.2(7)	25.6(5)	0.5(4)	2.2(4)	3.4(5)
Au24	42.0(7)	35.4(6)	48.4(7)	-6.6(5)	-4.4(5)	6.9(5)
S1	39(3)	28(3)	34(3)	5(2)	6(3)	6(3)
S2	32(3)	37(3)	32(3)	-3(2)	4(2)	3(3)
S3	35(3)	35(3)	29(3)	3(2)	5(2)	-3(3)
S4	35(3)	30(3)	22(3)	3(2)	3(2)	0(3)
S5	38(3)	31(3)	36(3)	-2(2)	4(3)	2(3)
S6	46(4)	47(4)	27(3)	-1(3)	4(3)	6(3)
S7	39(3)	34(3)	33(3)	-1(2)	0(3)	0(3)
S8	42(4)	46(4)	24(3)	5(2)	7(3)	6(3)
S9	39(4)	36(3)	46(4)	-1(3)	4(3)	0(3)
S10	38(4)	38(3)	41(4)	-1(3)	2(3)	3(3)
S11	45(4)	32(3)	36(3)	-4(2)	7(3)	1(3)
S12	36(3)	34(3)	36(3)	-1(2)	6(3)	5(3)
S13	52(4)	51(4)	23(3)	-7(3)	5(3)	-4(3)
S14	32(3)	43(4)	35(3)	0(3)	1(3)	0(3)
S15	46(4)	42(4)	40(4)	-9(3)	-2(3)	1(3)
S16	51(4)	57(4)	21(3)	-5(3)	3(3)	2(4)
C1	54(18)	30(13)	42(15)	-17(11)	3(13)	-1(13)
C2	46(16)	28(12)	32(13)	-9(10)	10(11)	-12(12)
C3	50(20)	60(20)	70(20)	-32(19)	-5(18)	7(17)
C4	50(16)	44(15)	25(13)	-13(11)	8(12)	-2(13)
C5	80(30)	35(17)	110(40)	-2(19)	30(30)	17(19)
C6	44(16)	49(17)	23(13)	1(11)	-22(11)	0(13)
C7	45(16)	21(11)	44(15)	-6(10)	9(12)	5(11)
C8	30(14)	60(20)	51(18)	16(15)	8(13)	6(14)
C9	48(17)	28(13)	48(16)	0(11)	-7(13)	17(13)
C10	60(20)	41(17)	50(20)	-6(14)	-15(16)	-9(16)
C11	30(15)	46(18)	90(30)	12(17)	9(16)	23(14)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	110(30)	30(15)	50(20)	-15(14)	0(20)	24(19)
C13	80(30)	39(16)	47(18)	29(14)	34(18)	22(17)
C14	52(19)	47(18)	52(19)	-6(14)	-1(15)	13(15)
C15	41(19)	47(19)	100(30)	10(19)	-8(19)	14(16)
C16	27(13)	60(20)	31(14)	-7(12)	-5(11)	10(13)
C17	80(30)	120(40)	24(16)	-7(18)	4(17)	-40(30)
C18	57(19)	21(12)	50(17)	3(11)	19(14)	-1(12)
C19	50(20)	130(40)	33(17)	-10(20)	2(15)	0(20)
C20	47(17)	40(16)	41(16)	-8(12)	1(13)	22(14)
C21	70(30)	50(20)	120(40)	40(30)	20(30)	0(20)
C22	54(18)	54(18)	30(14)	-13(12)	2(13)	19(15)
C23	48(19)	110(30)	38(17)	13(18)	24(15)	40(20)
C24	11(11)	63(19)	50(17)	-23(14)	7(10)	11(12)
C25	100(40)	34(18)	120(40)	-20(20)	60(30)	-10(20)
C26	100(30)	50(20)	50(20)	3(16)	-20(20)	-20(20)
C27	50(20)	90(30)	39(17)	-11(17)	11(15)	-2(19)
C28	34(15)	39(15)	80(20)	15(15)	29(16)	0(13)
C29	70(20)	80(30)	23(14)	-2(14)	-11(15)	-10(20)
C30	60(20)	70(20)	80(30)	60(20)	14(19)	27(19)
C31	48(19)	110(30)	25(15)	0(17)	-11(13)	0(20)
C32	80(30)	33(16)	70(20)	27(16)	10(20)	24(17)
C34	46(18)	60(20)	60(20)	4(16)	-6(16)	-2(16)
C33	48(18)	37(16)	70(20)	-4(14)	9(16)	-5(14)
C35	70(20)	110(30)	50(20)	30(20)	47(19)	20(20)
C36	50(20)	80(20)	42(17)	40(17)	18(15)	-9(18)
C37	70(20)	36(17)	100(30)	-21(18)	30(20)	16(17)
C38	70(20)	45(18)	60(20)	2(15)	1(18)	8(18)
C39	39(17)	60(20)	70(20)	-9(18)	-4(16)	14(16)
C40	53(18)	25(12)	41(15)	-13(10)	9(13)	6(13)
C41	70(30)	80(30)	33(17)	8(16)	9(16)	-10(20)
C42	50(20)	60(20)	90(30)	0(20)	-50(20)	-14(19)
C43	90(30)	50(20)	110(40)	10(20)	0(30)	30(20)
C44	70(20)	50(19)	45(18)	2(14)	9(17)	11(18)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C45	60(20)	30(15)	70(20)	-8(14)	10(19)	1(15)
C46	41(16)	55(18)	36(14)	-6(12)	3(12)	30(15)
C47	60(20)	60(20)	90(30)	20(20)	30(20)	40(20)
C48	80(30)	21(13)	80(20)	-19(14)	30(20)	-13(15)
C49	70(20)	90(30)	18(13)	8(14)	-7(14)	-30(20)
C50	70(20)	50(19)	60(20)	2(16)	30(19)	9(18)
C51	49(17)	40(15)	39(16)	-20(12)	14(13)	2(14)
C52	22(13)	90(30)	47(18)	-24(17)	0(12)	32(16)
C53	49(17)	40(14)	34(14)	-22(11)	28(12)	-15(13)
C54	70(30)	110(30)	18(14)	-15(17)	-9(15)	40(30)
C55	35(19)	110(40)	90(30)	-20(30)	-10(20)	-10(20)
C56	30(15)	90(30)	60(20)	30(20)	24(15)	29(18)
C57	60(20)	60(20)	60(20)	-4(17)	6(18)	22(18)
C58	50(20)	160(50)	34(18)	0(20)	-2(15)	-20(30)
C60	60(20)	48(18)	45(18)	-9(14)	-5(15)	11(16)
C61	60(20)	38(16)	60(20)	14(14)	-2(16)	31(15)
C62	90(40)	70(30)	110(40)	10(30)	50(30)	20(30)
C63	320(110)	80(30)	30(20)	0(20)	-10(40)	90(50)
C64	58(17)	35(13)	11(10)	7(9)	11(10)	-2(12)

Table S4. Bond Lengths for 20210518_008_Au24_bruker.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au1	Au2	2.9230(15)	Au17	S6	2.295(7)
Au1	Au3	3.2803(15)	Au18	Au20	3.3691(16)
Au1	Au4	2.7836(15)	Au18	Au21	3.1926(16)
Au1	Au5	2.8163(15)	Au18	S10	2.307(7)
Au1	Au6	2.7438(14)	Au18	S14	2.307(7)
Au1	Au7	2.6959(15)	Au19	S7	2.314(7)
Au1	Au8	2.7297(14)	Au19	S9	2.293(7)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au1	Au9	3.1039(14)	Au20	S10	2.319(8)
Au1	Au10	3.1493(15)	Au20	S11	2.301(8)
Au1	Au12	3.1661(15)	Au21	S12	2.316(7)
Au1	Au13	2.7574(15)	Au21	S14	2.309(7)
Au1	Au14	3.2757(15)	Au22	S6	2.302(8)
Au2	Au3	2.6945(15)	Au22	S13	2.297(8)
Au2	Au5	2.9144(14)	Au23	S8	2.289(8)
Au2	Au6	3.0114(16)	Au23	S16	2.289(8)
Au2	Au10	3.3615(16)	Au24	S9	2.310(8)
Au2	Au15	2.6821(15)	Au24	S15	2.318(8)
Au2	Au21	3.1235(17)	S1	C61	1.86(3)
Au2	S5	2.363(7)	S2	C20	1.86(3)
Au3	Au5	3.1382(15)	S3	C53	1.89(3)
Au3	Au7	2.9231(15)	S4	C2	1.85(3)
Au3	Au15	2.6369(14)	S5	C9	1.88(3)
Au3	Au18	3.1975(16)	S6	C51	1.91(3)
Au3	Au20	3.1569(15)	S7	C14	1.87(4)
Au3	Au21	3.0972(15)	S8	C24	1.82(3)
Au3	S4	2.406(6)	S9	C37	1.92(5)
Au4	Au6	2.7632(15)	S10	C57	1.88(4)
Au4	Au7	2.7471(16)	S11	C11	1.86(3)
Au4	Au9	2.9126(14)	S12	C40	1.85(3)
Au4	Au12	3.1995(15)	S13	C29	1.85(4)
Au4	S2	2.356(7)	S14	C16	1.90(3)
Au5	Au8	2.8043(15)	S15	C39	1.80(4)
Au5	Au13	2.7307(16)	S16	C6	1.81(3)
Au5	Au17	2.9618(15)	C1	C2	1.56(3)
Au5	Au21	3.3660(16)	C2	C7	1.46(4)
Au5	S12	2.386(7)	C2	C64	1.55(3)
Au6	Au7	2.7209(15)	C3	C24	1.56(5)
Au6	Au10	2.9155(15)	C4	C20	1.52(4)
Au6	Au23	3.0666(15)	C5	C11	1.46(6)
Au6	S8	2.364(6)	C6	C19	1.56(5)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au7	Au14	3.1545(15)	C6	C27	1.54(5)
Au7	Au15	3.2993(16)	C6	C33	1.56(4)
Au7	Au20	3.3655(16)	C8	C9	1.58(4)
Au7	S11	2.364(7)	C9	C30	1.50(5)
Au8	Au9	2.7605(16)	C9	C35	1.51(5)
Au8	Au13	2.7098(16)	C10	C57	1.53(5)
Au8	Au14	3.0385(15)	C11	C12	1.46(5)
Au8	Au16	2.8067(16)	C11	C62	1.65(6)
Au8	Au17	2.7976(16)	C13	C20	1.47(4)
Au8	Au22	2.8238(15)	C14	C38	1.59(5)
Au9	Au11	2.9226(16)	C14	C52	1.53(5)
Au9	Au12	2.7067(15)	C14	C56	1.47(5)
Au9	Au14	3.2802(16)	C15	C16	1.53(5)
Au9	Au16	2.7238(15)	C16	C50	1.47(5)
Au9	S1	2.370(7)	C16	C54	1.54(4)
Au10	Au13	2.9542(15)	C17	C29	1.48(5)
Au10	S3	2.323(7)	C18	C53	1.46(4)
Au10	S5	2.312(7)	C20	C46	1.49(4)
Au11	Au12	3.1783(15)	C21	C61	1.48(6)
Au11	Au19	3.2368(15)	C22	C40	1.48(5)
Au11	S2	2.296(7)	C23	C24	1.59(4)
Au11	S7	2.330(7)	C24	C41	1.51(5)
Au12	Au13	2.9076(16)	C25	C37	1.51(5)
Au12	Au16	2.6419(15)	C26	C37	1.46(6)
Au12	Au19	3.1649(15)	C28	C53	1.51(5)
Au12	Au24	3.2756(16)	C29	C32	1.56(6)
Au12	S3	2.359(6)	C29	C58	1.44(6)
Au13	Au16	3.2477(15)	C31	C51	1.52(4)
Au13	Au24	3.3270(17)	C34	C51	1.52(5)
Au13	S15	2.368(7)	C36	C51	1.52(5)
Au14	S1	2.307(7)	C37	C55	1.43(6)
Au14	S4	2.304(7)	C39	C43	1.57(6)
Au15	Au18	2.9192(17)	C39	C48	1.55(5)

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Au15	Au20	3.0160(16)	C39	C60	1.58(6)
Au15	Au23	2.9545(16)	C40	C44	1.45(5)
Au15	S16	2.377(7)	C40	C47	1.57(5)
Au16	Au19	2.9180(17)	C42	C57	1.43(6)
Au16	Au22	3.2935(17)	C45	C53	1.50(4)
Au16	Au24	3.0478(17)	C49	C57	1.49(5)
Au16	S13	2.370(7)	C59	C61	1.63(6)
Au17	S4	2.321(6)	C61	C63	1.34(6)

Table S5. Bond Angles for 20210518_008_Au24_bruker.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Au2	Au1	Au3	51.09(3)	S3	Au12	Au1	86.29(17)
Au2	Au1	Au9	176.24(5)	S3	Au12	Au4	73.52(17)
Au2	Au1	Au10	67.10(4)	S3	Au12	Au9	131.84(17)
Au2	Au1	Au12	132.27(5)	S3	Au12	Au11	103.90(17)
Au2	Au1	Au14	114.60(4)	S3	Au12	Au13	96.96(17)
Au4	Au1	Au2	123.02(4)	S3	Au12	Au16	164.28(17)
Au4	Au1	Au3	117.71(4)	S3	Au12	Au19	122.38(17)
Au4	Au1	Au5	174.72(5)	S3	Au12	Au24	104.91(17)
Au4	Au1	Au9	59.00(3)	Au1	Au13	Au10	66.82(4)
Au4	Au1	Au10	92.22(4)	Au1	Au13	Au12	67.90(4)
Au4	Au1	Au12	64.69(4)	Au1	Au13	Au16	90.76(4)
Au4	Au1	Au14	87.64(4)	Au1	Au13	Au24	130.75(5)
Au5	Au1	Au2	61.00(4)	Au5	Au13	Au1	61.75(4)
Au5	Au1	Au3	61.40(4)	Au5	Au13	Au10	98.87(5)
Au5	Au1	Au9	116.77(4)	Au5	Au13	Au12	128.06(5)
Au5	Au1	Au10	92.66(4)	Au5	Au13	Au16	117.07(5)
Au5	Au1	Au12	115.74(4)	Au5	Au13	Au24	161.14(5)
Au5	Au1	Au14	87.42(4)	Au8	Au13	Au1	59.90(4)
Au6	Au1	Au2	64.11(4)	Au8	Au13	Au5	62.05(4)
Au6	Au1	Au3	89.76(4)	Au8	Au13	Au10	126.27(5)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Au6	Au1	Au4	59.98(4)	Au8	Au13	Au12	82.75(4)
Au6	Au1	Au5	124.59(5)	Au8	Au13	Au16	55.33(4)
Au6	Au1	Au9	118.44(5)	Au8	Au13	Au24	109.40(5)
Au6	Au1	Au10	58.82(4)	Au10	Au13	Au16	121.73(5)
Au6	Au1	Au12	95.38(4)	Au10	Au13	Au24	99.47(5)
Au6	Au1	Au13	118.40(5)	Au12	Au13	Au10	71.31(4)
Au6	Au1	Au14	122.66(4)	Au12	Au13	Au16	50.46(3)
Au7	Au1	Au2	83.56(4)	Au12	Au13	Au24	62.97(4)
Au7	Au1	Au3	57.58(4)	Au16	Au13	Au24	55.22(3)
Au7	Au1	Au4	60.15(4)	S15	Au13	Au1	171.2(2)
Au7	Au1	Au5	118.84(5)	S15	Au13	Au5	121.1(2)
Au7	Au1	Au6	60.02(4)	S15	Au13	Au8	113.1(2)
Au7	Au1	Au8	122.84(5)	S15	Au13	Au10	119.1(2)
Au7	Au1	Au9	95.37(4)	S15	Au13	Au12	106.9(2)
Au7	Au1	Au10	118.70(4)	S15	Au13	Au16	80.53(19)
Au7	Au1	Au12	124.73(5)	S15	Au13	Au24	44.2(2)
Au7	Au1	Au13	176.15(6)	Au1	Au14	Au9	56.52(3)
Au7	Au1	Au14	62.89(4)	Au7	Au14	Au1	49.53(3)
Au8	Au1	Au2	121.65(5)	Au7	Au14	Au9	83.78(4)
Au8	Au1	Au3	97.10(4)	Au8	Au14	Au1	51.06(3)
Au8	Au1	Au4	114.97(5)	Au8	Au14	Au7	100.57(4)
Au8	Au1	Au5	60.72(4)	Au8	Au14	Au9	51.64(3)
Au8	Au1	Au6	172.99(6)	S1	Au14	Au1	93.37(16)
Au8	Au1	Au9	56.04(4)	S1	Au14	Au7	87.29(16)
Au8	Au1	Au10	118.38(5)	S1	Au14	Au8	95.73(17)
Au8	Au1	Au12	77.75(4)	S1	Au14	Au9	46.26(16)
Au8	Au1	Au13	59.19(4)	S4	Au14	Au1	90.45(15)
Au8	Au1	Au14	59.97(4)	S4	Au14	Au7	95.62(14)
Au9	Au1	Au3	125.37(4)	S4	Au14	Au8	86.24(16)
Au9	Au1	Au10	116.46(4)	S4	Au14	Au9	136.49(16)
Au9	Au1	Au12	51.14(3)	S4	Au14	S1	176.1(2)
Au9	Au1	Au14	61.81(3)	Au2	Au15	Au7	76.82(4)
Au10	Au1	Au3	118.17(4)	Au2	Au15	Au18	103.95(5)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Au10	Au1	Au12	65.52(3)	Au2	Au15	Au20	126.48(5)
Au10	Au1	Au14	178.01(5)	Au2	Au15	Au23	94.78(5)
Au12	Au1	Au3	174.81(4)	Au3	Au15	Au2	60.87(4)
Au12	Au1	Au14	112.68(4)	Au3	Au15	Au7	57.71(4)
Au13	Au1	Au2	92.59(4)	Au3	Au15	Au18	70.06(4)
Au13	Au1	Au3	119.63(5)	Au3	Au15	Au20	67.51(4)
Au13	Au1	Au4	122.64(5)	Au3	Au15	Au23	139.70(5)
Au13	Au1	Au5	58.66(4)	Au18	Au15	Au7	119.35(5)
Au13	Au1	Au9	88.46(4)	Au18	Au15	Au20	69.15(4)
Au13	Au1	Au10	59.58(4)	Au18	Au15	Au23	150.23(5)
Au13	Au1	Au12	58.31(4)	Au20	Au15	Au7	64.22(4)
Au13	Au1	Au14	118.91(4)	Au23	Au15	Au7	87.11(4)
Au14	Au1	Au3	63.58(3)	Au23	Au15	Au20	117.13(5)
Au1	Au2	Au6	55.05(3)	S16	Au15	Au2	136.3(2)
Au1	Au2	Au10	59.66(3)	S16	Au15	Au3	162.6(2)
Au1	Au2	Au21	118.67(4)	S16	Au15	Au7	117.9(2)
Au3	Au2	Au1	71.32(4)	S16	Au15	Au18	102.6(2)
Au3	Au2	Au5	67.91(4)	S16	Au15	Au20	95.3(2)
Au3	Au2	Au6	96.66(4)	S16	Au15	Au23	49.4(2)
Au3	Au2	Au10	130.94(5)	Au8	Au16	Au13	52.56(4)
Au3	Au2	Au21	63.83(4)	Au8	Au16	Au19	151.93(5)
Au5	Au2	Au1	57.69(3)	Au8	Au16	Au22	54.44(4)
Au5	Au2	Au6	112.34(4)	Au8	Au16	Au24	115.02(5)
Au5	Au2	Au10	86.72(4)	Au9	Au16	Au8	59.87(4)
Au5	Au2	Au21	67.66(4)	Au9	Au16	Au13	86.15(4)
Au6	Au2	Au10	54.11(3)	Au9	Au16	Au19	95.40(5)
Au6	Au2	Au21	159.53(5)	Au9	Au16	Au22	105.50(5)
Au15	Au2	Au1	104.53(5)	Au9	Au16	Au24	130.30(5)
Au15	Au2	Au3	58.74(4)	Au12	Au16	Au8	85.94(4)
Au15	Au2	Au5	126.58(5)	Au12	Au16	Au9	60.57(4)
Au15	Au2	Au6	77.86(4)	Au12	Au16	Au13	58.08(4)
Au15	Au2	Au10	130.46(5)	Au12	Au16	Au19	69.19(4)
Au15	Au2	Au21	86.07(4)	Au12	Au16	Au22	135.87(5)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Au21	Au2	Au10	143.46(5)	Au12	Au16	Au24	69.88(4)
S5	Au2	Au1	94.87(17)	Au13	Au16	Au22	80.58(4)
S5	Au2	Au3	152.46(17)	Au19	Au16	Au13	117.84(5)
S5	Au2	Au5	84.55(17)	Au19	Au16	Au22	153.32(5)
S5	Au2	Au6	94.21(17)	Au19	Au16	Au24	69.31(4)
S5	Au2	Au10	43.41(17)	Au24	Au16	Au13	63.71(4)
S5	Au2	Au15	148.70(17)	Au24	Au16	Au22	107.07(5)
S5	Au2	Au21	106.04(18)	S13	Au16	Au8	98.6(2)
Au2	Au3	Au1	57.58(4)	S13	Au16	Au9	137.4(2)
Au2	Au3	Au5	59.38(3)	S13	Au16	Au12	160.9(2)
Au2	Au3	Au7	83.58(4)	S13	Au16	Au13	110.4(2)
Au2	Au3	Au18	96.69(4)	S13	Au16	Au19	109.1(2)
Au2	Au3	Au20	120.68(5)	S13	Au16	Au22	44.2(2)
Au2	Au3	Au21	64.84(4)	S13	Au16	Au24	91.5(2)
Au5	Au3	Au1	51.99(3)	Au8	Au17	Au5	58.19(4)
Au5	Au3	Au18	126.27(4)	S4	Au17	Au5	79.90(15)
Au5	Au3	Au20	169.49(5)	S4	Au17	Au8	91.81(17)
Au7	Au3	Au1	51.12(3)	S6	Au17	Au5	105.3(2)
Au7	Au3	Au5	103.01(4)	S6	Au17	Au8	89.8(2)
Au7	Au3	Au18	122.63(4)	S6	Au17	S4	174.6(2)
Au7	Au3	Au20	67.09(4)	Au3	Au18	Au20	57.40(3)
Au7	Au3	Au21	148.14(5)	Au15	Au18	Au3	50.83(3)
Au15	Au3	Au1	96.50(4)	Au15	Au18	Au20	56.78(4)
Au15	Au3	Au2	60.40(4)	Au15	Au18	Au21	81.01(4)
Au15	Au3	Au5	119.71(5)	Au21	Au18	Au3	57.98(3)
Au15	Au3	Au7	72.59(4)	Au21	Au18	Au20	115.33(5)
Au15	Au3	Au18	59.12(4)	S10	Au18	Au3	86.51(18)
Au15	Au3	Au20	61.97(4)	S10	Au18	Au15	100.0(2)
Au15	Au3	Au21	87.39(4)	S10	Au18	Au20	43.39(19)
Au18	Au3	Au1	152.52(4)	S10	Au18	Au21	133.50(19)
Au20	Au3	Au1	118.21(4)	S14	Au18	Au3	93.72(17)
Au20	Au3	Au18	64.03(4)	S14	Au18	Au15	80.72(18)
Au21	Au3	Au1	109.28(4)	S14	Au18	Au20	137.27(18)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Au21	Au3	Au5	65.34(4)	S14	Au18	Au21	46.26(17)
Au21	Au3	Au18	60.93(4)	S14	Au18	S10	179.3(3)
Au21	Au3	Au20	124.90(5)	Au12	Au19	Au11	59.52(3)
S4	Au3	Au1	88.58(16)	Au16	Au19	Au11	84.73(4)
S4	Au3	Au2	133.63(15)	Au16	Au19	Au12	51.29(3)
S4	Au3	Au5	75.07(15)	S7	Au19	Au11	46.01(17)
S4	Au3	Au7	99.61(16)	S7	Au19	Au12	95.53(17)
S4	Au3	Au15	164.17(15)	S7	Au19	Au16	85.45(19)
S4	Au3	Au18	118.37(16)	S9	Au19	Au11	135.2(2)
S4	Au3	Au20	102.43(15)	S9	Au19	Au12	88.54(19)
S4	Au3	Au21	105.12(16)	S9	Au19	Au16	99.6(2)
Au1	Au4	Au9	65.99(4)	S9	Au19	S7	174.9(3)
Au1	Au4	Au12	63.45(4)	Au3	Au20	Au7	53.13(3)
Au6	Au4	Au1	59.29(4)	Au3	Au20	Au18	58.57(3)
Au6	Au4	Au9	124.67(5)	Au7	Au20	Au18	105.79(4)
Au6	Au4	Au12	94.24(4)	Au15	Au20	Au3	50.51(3)
Au7	Au4	Au1	58.34(4)	Au15	Au20	Au7	61.98(4)
Au7	Au4	Au6	59.18(4)	Au15	Au20	Au18	54.07(4)
Au7	Au4	Au9	98.76(5)	S10	Au20	Au3	87.29(18)
Au7	Au4	Au12	121.69(5)	S10	Au20	Au7	140.31(18)
Au9	Au4	Au12	52.31(3)	S10	Au20	Au15	96.99(18)
S2	Au4	Au1	150.25(17)	S10	Au20	Au18	43.12(18)
S2	Au4	Au6	128.39(17)	S11	Au20	Au3	97.55(17)
S2	Au4	Au7	151.21(17)	S11	Au20	Au7	44.57(17)
S2	Au4	Au9	96.04(16)	S11	Au20	Au15	85.60(18)
S2	Au4	Au12	86.81(16)	S11	Au20	Au18	139.67(18)
Au1	Au5	Au2	61.31(4)	S11	Au20	S10	175.1(3)
Au1	Au5	Au3	66.60(4)	Au2	Au21	Au5	53.21(3)
Au1	Au5	Au17	101.98(4)	Au2	Au21	Au18	88.69(4)
Au1	Au5	Au21	114.29(4)	Au3	Au21	Au2	51.33(3)
Au2	Au5	Au3	52.71(3)	Au3	Au21	Au5	57.92(3)
Au2	Au5	Au17	136.83(5)	Au3	Au21	Au18	61.09(4)
Au2	Au5	Au21	59.13(4)	Au18	Au21	Au5	119.00(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Au3	Au5	Au21	56.74(3)	S12	Au21	Au2	97.77(18)
Au8	Au5	Au1	58.11(4)	S12	Au21	Au3	89.50(17)
Au8	Au5	Au2	119.34(5)	S12	Au21	Au5	45.13(18)
Au8	Au5	Au3	98.86(4)	S12	Au21	Au18	135.83(18)
Au8	Au5	Au17	57.97(4)	S14	Au21	Au2	88.59(18)
Au8	Au5	Au21	152.17(5)	S14	Au21	Au3	96.35(18)
Au13	Au5	Au1	59.59(4)	S14	Au21	Au5	141.49(18)
Au13	Au5	Au2	93.33(4)	S14	Au21	Au18	46.21(18)
Au13	Au5	Au3	125.70(5)	S14	Au21	S12	173.2(3)
Au13	Au5	Au8	58.61(4)	Au8	Au22	Au16	53.96(4)
Au13	Au5	Au17	112.61(5)	S6	Au22	Au8	89.02(17)
Au13	Au5	Au21	144.76(5)	S6	Au22	Au16	142.67(17)
Au17	Au5	Au3	84.24(4)	S13	Au22	Au8	99.92(17)
Au17	Au5	Au21	102.62(4)	S13	Au22	Au16	46.01(16)
S12	Au5	Au1	153.82(17)	S13	Au22	S6	170.6(2)
S12	Au5	Au2	101.99(17)	Au15	Au23	Au6	73.10(4)
S12	Au5	Au3	87.28(17)	S8	Au23	Au6	49.84(16)
S12	Au5	Au8	132.27(17)	S8	Au23	Au15	121.81(16)
S12	Au5	Au13	145.77(17)	S16	Au23	Au6	123.86(17)
S12	Au5	Au17	75.91(17)	S16	Au23	Au15	52.05(17)
S12	Au5	Au21	43.46(17)	S16	Au23	S8	173.7(2)
Au1	Au6	Au2	60.84(4)	Au12	Au24	Au13	52.25(3)
Au1	Au6	Au4	60.72(4)	Au16	Au24	Au12	49.23(3)
Au1	Au6	Au10	67.55(4)	Au16	Au24	Au13	61.07(4)
Au1	Au6	Au23	139.89(5)	S9	Au24	Au12	85.61(19)
Au2	Au6	Au23	86.18(4)	S9	Au24	Au13	137.76(19)
Au4	Au6	Au2	120.54(5)	S9	Au24	Au16	95.61(19)
Au4	Au6	Au10	97.88(4)	S9	Au24	S15	176.8(3)
Au4	Au6	Au23	137.25(5)	S15	Au24	Au12	97.46(18)
Au7	Au6	Au1	59.12(4)	S15	Au24	Au13	45.37(18)
Au7	Au6	Au2	81.48(4)	S15	Au24	Au16	85.8(2)
Au7	Au6	Au4	60.12(4)	Au14	S1	Au9	89.1(2)
Au7	Au6	Au10	126.50(5)	C61	S1	Au9	111.5(12)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Au7	Au6	Au23	96.27(5)	C61	S1	Au14	105.0(12)
Au10	Au6	Au2	69.08(4)	Au11	S2	Au4	94.1(2)
Au10	Au6	Au23	123.85(5)	C20	S2	Au4	111.7(11)
S8	Au6	Au1	167.43(19)	C20	S2	Au11	104.9(10)
S8	Au6	Au2	116.94(18)	Au10	S3	Au12	93.8(2)
S8	Au6	Au4	122.47(18)	C53	S3	Au10	109.9(10)
S8	Au6	Au7	133.45(18)	C53	S3	Au12	117.1(9)
S8	Au6	Au10	99.93(18)	Au14	S4	Au3	94.3(2)
S8	Au6	Au23	47.73(18)	Au14	S4	Au17	95.7(2)
Au1	Au7	Au3	71.30(4)	Au17	S4	Au3	120.0(3)
Au1	Au7	Au4	61.51(4)	C2	S4	Au3	118.5(9)
Au1	Au7	Au6	60.87(4)	C2	S4	Au14	115.1(10)
Au1	Au7	Au14	67.57(4)	C2	S4	Au17	109.7(9)
Au1	Au7	Au15	94.90(4)	Au10	S5	Au2	91.9(2)
Au1	Au7	Au20	131.08(5)	C9	S5	Au2	107.0(10)
Au3	Au7	Au14	69.14(4)	C9	S5	Au10	110.6(11)
Au3	Au7	Au15	49.70(3)	Au17	S6	Au22	100.9(3)
Au3	Au7	Au20	59.77(4)	C51	S6	Au17	107.1(9)
Au4	Au7	Au3	132.79(5)	C51	S6	Au22	102.9(11)
Au4	Au7	Au14	90.76(4)	Au19	S7	Au11	88.4(2)
Au4	Au7	Au15	133.08(5)	C14	S7	Au11	108.5(12)
Au4	Au7	Au20	167.33(5)	C14	S7	Au19	107.3(12)
Au6	Au7	Au3	98.18(5)	Au23	S8	Au6	82.4(2)
Au6	Au7	Au4	60.71(4)	C24	S8	Au6	107.6(12)
Au6	Au7	Au14	128.15(5)	C24	S8	Au23	104.7(10)
Au6	Au7	Au15	72.41(4)	Au19	S9	Au24	95.0(3)
Au6	Au7	Au20	124.04(5)	C37	S9	Au19	108.1(13)
Au14	Au7	Au15	118.55(4)	C37	S9	Au24	108.3(12)
Au14	Au7	Au20	93.55(4)	Au18	S10	Au20	93.5(3)
Au15	Au7	Au20	53.80(3)	C57	S10	Au18	106.5(13)
S11	Au7	Au1	173.06(19)	C57	S10	Au20	106.6(13)
S11	Au7	Au3	102.70(19)	Au20	S11	Au7	92.3(2)
S11	Au7	Au4	124.49(19)	C11	S11	Au7	113.7(14)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S11	Au7	Au6	117.75(18)	C11	S11	Au20	107.7(12)
S11	Au7	Au14	114.09(18)	Au21	S12	Au5	91.4(2)
S11	Au7	Au15	78.36(18)	C40	S12	Au5	109.7(11)
S11	Au7	Au20	43.09(19)	C40	S12	Au21	106.7(10)
Au1	Au8	Au5	61.17(4)	Au22	S13	Au16	89.8(2)
Au1	Au8	Au9	68.85(4)	C29	S13	Au16	110.1(13)
Au1	Au8	Au14	68.97(4)	C29	S13	Au22	106.8(13)
Au1	Au8	Au16	101.51(5)	Au18	S14	Au21	87.5(2)
Au1	Au8	Au17	108.68(5)	C16	S14	Au18	107.8(11)
Au1	Au8	Au22	160.54(6)	C16	S14	Au21	108.0(9)
Au5	Au8	Au14	92.47(4)	Au24	S15	Au13	90.5(3)
Au5	Au8	Au16	131.03(5)	C39	S15	Au13	111.5(13)
Au5	Au8	Au22	109.00(5)	C39	S15	Au24	109.3(13)
Au9	Au8	Au5	130.02(5)	Au23	S16	Au15	78.5(2)
Au9	Au8	Au14	68.70(4)	C6	S16	Au15	114.6(11)
Au9	Au8	Au16	58.58(4)	C6	S16	Au23	106.6(11)
Au9	Au8	Au17	138.31(5)	C1	C2	S4	108(2)
Au9	Au8	Au22	118.61(5)	C7	C2	S4	109(2)
Au13	Au8	Au1	60.92(4)	C7	C2	C1	112(2)
Au13	Au8	Au5	59.34(4)	C7	C2	C64	112(2)
Au13	Au8	Au9	96.96(5)	C64	C2	S4	108.8(19)
Au13	Au8	Au14	129.58(5)	C64	C2	C1	106(2)
Au13	Au8	Au16	72.11(4)	C19	C6	S16	106(3)
Au13	Au8	Au17	118.69(5)	C19	C6	C33	107(3)
Au13	Au8	Au22	99.70(5)	C27	C6	S16	111(2)
Au16	Au8	Au14	125.61(5)	C27	C6	C19	111(3)
Au16	Au8	Au22	71.60(4)	C27	C6	C33	110(3)
Au17	Au8	Au5	63.84(4)	C33	C6	S16	112(2)
Au17	Au8	Au14	71.85(4)	C8	C9	S5	105(2)
Au17	Au8	Au16	149.39(5)	C30	C9	S5	107(2)
Au17	Au8	Au22	78.17(4)	C30	C9	C8	110(3)
Au22	Au8	Au14	130.06(5)	C30	C9	C35	114(3)
Au1	Au9	Au14	61.67(3)	C35	C9	S5	111(2)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Au4	Au9	Au1	55.01(3)	C35	C9	C8	110(3)
Au4	Au9	Au11	71.43(4)	C5	C11	S11	114(3)
Au4	Au9	Au14	85.45(4)	C5	C11	C62	111(4)
Au8	Au9	Au1	55.10(3)	C12	C11	S11	107(3)
Au8	Au9	Au4	110.04(5)	C12	C11	C5	109(4)
Au8	Au9	Au11	152.17(5)	C12	C11	C62	112(4)
Au8	Au9	Au14	59.66(4)	C62	C11	S11	105(3)
Au11	Au9	Au1	118.22(4)	C38	C14	S7	104(3)
Au11	Au9	Au14	145.58(5)	C52	C14	S7	104(2)
Au12	Au9	Au1	65.62(4)	C52	C14	C38	108(3)
Au12	Au9	Au4	69.30(4)	C56	C14	S7	113(2)
Au12	Au9	Au8	85.63(4)	C56	C14	C38	111(3)
Au12	Au9	Au11	68.62(4)	C56	C14	C52	116(3)
Au12	Au9	Au14	126.91(5)	C15	C16	S14	103(2)
Au12	Au9	Au16	58.22(4)	C15	C16	C54	112(3)
Au16	Au9	Au1	94.53(4)	C50	C16	S14	111(2)
Au16	Au9	Au4	127.02(5)	C50	C16	C15	110(3)
Au16	Au9	Au8	61.56(4)	C50	C16	C54	115(3)
Au16	Au9	Au11	94.67(5)	C54	C16	S14	105(2)
Au16	Au9	Au14	119.73(5)	C4	C20	S2	105(2)
S1	Au9	Au1	96.58(17)	C13	C20	S2	112(2)
S1	Au9	Au4	82.95(16)	C13	C20	C4	115(3)
S1	Au9	Au8	101.97(17)	C13	C20	C46	110(3)
S1	Au9	Au11	105.74(17)	C46	C20	S2	107(2)
S1	Au9	Au12	152.12(16)	C46	C20	C4	108(3)
S1	Au9	Au14	44.68(17)	C3	C24	S8	115(2)
S1	Au9	Au16	148.44(17)	C3	C24	C23	106(3)
Au1	Au10	Au2	53.23(3)	C23	C24	S8	109(2)
Au6	Au10	Au1	53.63(3)	C41	C24	S8	108(2)
Au6	Au10	Au2	56.81(3)	C41	C24	C3	110(3)
Au6	Au10	Au13	107.23(4)	C41	C24	C23	108(3)
Au13	Au10	Au1	53.60(3)	C17	C29	S13	111(3)
Au13	Au10	Au2	80.87(4)	C17	C29	C32	108(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S3	Au10	Au1	87.29(16)	C32	C29	S13	111(2)
S3	Au10	Au2	132.75(17)	C58	C29	S13	104(3)
S3	Au10	Au6	79.92(17)	C58	C29	C17	110(3)
S3	Au10	Au13	96.51(16)	C58	C29	C32	113(4)
S5	Au10	Au1	90.16(17)	C25	C37	S9	109(4)
S5	Au10	Au2	44.64(16)	C26	C37	S9	109(3)
S5	Au10	Au6	97.90(17)	C26	C37	C25	109(3)
S5	Au10	Au13	82.60(17)	C55	C37	S9	104(3)
S5	Au10	S3	177.3(2)	C55	C37	C25	110(4)
Au9	Au11	Au12	52.47(3)	C55	C37	C26	116(5)
Au9	Au11	Au19	85.19(4)	C43	C39	S15	109(3)
Au12	Au11	Au19	59.11(3)	C43	C39	C60	111(4)
S2	Au11	Au9	97.13(18)	C48	C39	S15	107(3)
S2	Au11	Au12	88.33(17)	C48	C39	C43	108(3)
S2	Au11	Au19	136.75(17)	C48	C39	C60	108(3)
S2	Au11	S7	176.8(2)	C60	C39	S15	113(2)
S7	Au11	Au9	85.06(19)	C22	C40	S12	113(2)
S7	Au11	Au12	94.85(18)	C22	C40	C47	109(3)
S7	Au11	Au19	45.61(17)	C44	C40	S12	108(2)
Au1	Au12	Au4	51.86(3)	C44	C40	C22	110(3)
Au1	Au12	Au11	109.23(4)	C44	C40	C47	110(3)
Au1	Au12	Au24	118.50(4)	C47	C40	S12	106(2)
Au4	Au12	Au24	170.01(5)	C31	C51	S6	108(2)
Au9	Au12	Au1	63.24(4)	C34	C51	S6	112(2)
Au9	Au12	Au4	58.38(3)	C34	C51	C31	115(3)
Au9	Au12	Au11	58.90(4)	C36	C51	S6	104(2)
Au9	Au12	Au13	93.63(5)	C36	C51	C31	108(3)
Au9	Au12	Au19	90.29(4)	C36	C51	C34	109(3)
Au9	Au12	Au24	121.98(5)	C18	C53	S3	102.8(19)
Au11	Au12	Au4	64.56(3)	C18	C53	C28	111(3)
Au11	Au12	Au24	124.95(4)	C18	C53	C45	112(3)
Au13	Au12	Au1	53.79(3)	C28	C53	S3	106(2)
Au13	Au12	Au4	105.40(4)	C45	C53	S3	112(2)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Au13	Au12	Au11	152.36(5)	C45	C53	C28	113(3)
Au13	Au12	Au19	120.87(5)	C10	C57	S10	104(3)
Au13	Au12	Au24	64.79(4)	C42	C57	S10	107(3)
Au16	Au12	Au1	94.74(4)	C42	C57	C10	111(4)
Au16	Au12	Au4	119.16(5)	C42	C57	C49	111(4)
Au16	Au12	Au9	61.21(4)	C49	C57	S10	111(3)
Au16	Au12	Au11	90.60(4)	C49	C57	C10	112(4)
Au16	Au12	Au13	71.46(4)	C21	C61	S1	107(3)
Au16	Au12	Au19	59.52(4)	C21	C61	C59	108(3)
Au16	Au12	Au24	60.89(4)	C59	C61	S1	103(3)
Au19	Au12	Au1	150.71(5)	C63	C61	S1	113(3)
Au19	Au12	Au4	125.83(4)	C63	C61	C21	123(5)
Au19	Au12	Au11	61.37(3)	C63	C61	C59	101(5)
Au19	Au12	Au24	63.58(4)				

Table S6. Torsion Angles for 20210518_008_Au24_bruker.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Au2	S5	C9	C8	-57(2)	Au14	S1	C61	C63	49(5)
Au2	S5	C9	C30	-174(2)	Au14	S4	C2	C1	43(2)
Au2	S5	C9	C35	61(3)	Au14	S4	C2	C7	165.8(16)
Au3	S4	C2	C1	-67(2)	Au14	S4	C2	C64	-72(2)
Au3	S4	C2	C7	55(2)	Au15	S16	C6	C19	-157(2)
Au3	S4	C2	C64	177.4(16)	Au15	S16	C6	C27	83(2)
Au4	S2	C20	C4	-74(2)	Au15	S16	C6	C33	-41(3)
Au4	S2	C20	C13	51(3)	Au16	S13	C29	C17	161(2)
Au4	S2	C20	C46	171.4(18)	Au16	S13	C29	C32	41(3)
Au5	S12	C40	C22	-53(2)	Au16	S13	C29	C58	-81(3)
Au5	S12	C40	C44	69(3)	Au17	S4	C2	C1	149.6(18)
Au5	S12	C40	C47	-173(2)	Au17	S4	C2	C7	-87.6(19)
Au6	S8	C24	C3	-46(2)	Au17	S4	C2	C64	34(2)
Au6	S8	C24	C23	-164(2)	Au18	S10	C57	C10	-176(2)

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Au6	S8	C24	C41	78(2)	Au18	S10	C57	C42	66(3)
Au7	S11	C11	C5	-57(3)	Au18	S10	C57	C49	-56(3)
Au7	S11	C11	C12	-177(3)	Au19	S7	C14	C38	163(2)
Au7	S11	C11	C62	64(3)	Au19	S7	C14	C52	-84(3)
Au9	S1	C61	C21	175(3)	Au19	S7	C14	C56	42(3)
Au9	S1	C61	C59	62(2)	Au20	S10	C57	C10	-77(3)
Au9	S1	C61	C63	-46(5)	Au20	S10	C57	C42	165(3)
Au10	S3	C53	C18	81(2)	Au20	S10	C57	C49	43(3)
Au10	S3	C53	C28	-162.5(18)	Au20	S11	C11	C5	44(3)
Au10	S3	C53	C45	-39(3)	Au20	S11	C11	C12	-77(3)
Au10	S5	C9	C8	-156.1(18)	Au20	S11	C11	C62	165(3)
Au10	S5	C9	C30	87(2)	Au21	S12	C40	C22	45(2)
Au10	S5	C9	C35	-37(3)	Au21	S12	C40	C44	167(2)
Au11	S2	C20	C4	-174.5(19)	Au21	S12	C40	C47	-75(2)
Au11	S2	C20	C13	-50(3)	Au22	S13	C29	C17	65(3)
Au11	S2	C20	C46	71(2)	Au22	S13	C29	C32	-55(3)
Au11	S7	C14	C38	68(3)	Au22	S13	C29	C58	-177(3)
Au11	S7	C14	C52	-178(2)	Au23	S8	C24	C3	41(2)
Au11	S7	C14	C56	-52(3)	Au23	S8	C24	C23	-78(3)
Au12	S3	C53	C18	-173.5(17)	Au23	S8	C24	C41	165(2)
Au12	S3	C53	C28	-57(2)	Au23	S16	C6	C19	-72(3)
Au12	S3	C53	C45	66(3)	Au23	S16	C6	C27	168(2)
Au13	S15	C39	C43	-69(3)	Au23	S16	C6	C33	44(3)
Au13	S15	C39	C48	175(2)	Au24	S15	C39	C43	-167(3)
Au13	S15	C39	C60	55(3)	Au24	S15	C39	C48	76(3)
Au14	S1	C61	C21	-90(3)	Au24	S15	C39	C60	-43(3)
Au14	S1	C61	C59	157(2)					

Table S7. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 20210518_008_Au24_bruker.

Atom	***x***	***y***	***z***	**U(eq)**
H1A	6525.36	5909.29	4462.33	64
H1B	7498.67	6126.65	4510.86	64
H1C	7247.51	5756.99	4897.33	64
H3A	3297	4876.72	6577.72	93
H3B	3896.68	4718.05	6217.87	93
H3C	4324.57	4798.91	6744.74	93
H4A	1866.75	5658.71	5754.51	59
H4B	2581.08	5212.14	5772.95	59
H4C	1634.66	5080.3	5877.3	59
H5A	5972.27	6299.75	5243.83	109
H5B	5047.07	6577.31	5093.23	109
H5C	5152.53	5978.72	4983.35	109
H7A	8370.88	5035.07	4764.61	55
H7B	8683.56	5503.36	4483.64	55
H7C	8479.4	4952.36	4245.2	55
H8A	7613.9	2145.47	5925	71
H8B	7513.35	2421.83	6393.3	71
H8C	7463.36	2755.7	5936.87	71
H10A	9169.69	6483.46	5934.76	83
H10B	9034.71	6549.9	6451.73	83
H10C	8222.54	6406.11	6059.14	83
H12A	5161.25	6479.34	6245.29	97
H12B	5352.25	6851.54	5846.19	97
H12C	6082.32	6452.99	6082.24	97
H13A	1754.09	5427.92	4561.12	80
H13B	2603.11	5534.62	4942.3	80
H13C	1754.31	5887.56	4920.17	80
H15A	9876.45	2810.9	6251.19	98
H15B	10641.8	2869.87	5963.16	98
H15C	9644.33	2876.11	5707.54	98
H17A	2855.47	4126.27	1788.04	113
H17B	2946.42	3511.92	1823.15	113
H17C	3745.48	3871.84	2047.45	113

Atom	*x*	*y*	*z*	U(eq)
H18A	2046.71	2789.49	5855.37	62
H18B	3004.94	2556.13	5882.25	62
H18C	2176.1	2180.65	5808.33	62
H19A	7877.04	4350.35	7849	108
H19B	7765.3	3736.61	7826.71	108
H19C	6952.06	4101.71	7635.4	108
H21A	3810.81	6402.69	3548.85	122
H21B	4390.56	6221.1	4023.34	122
H21C	3379.28	6352.72	3994.75	122
H22A	8100.79	2505.58	4965.12	70
H22B	7944.3	2060.52	4586.08	70
H22C	7158.93	2434.24	4650.16	70
H23A	3369.58	4349.28	7263.82	97
H23B	4280.97	4049.52	7325.12	97
H23C	3384.23	3733.39	7227.96	97
H25A	486.56	1438.17	3018.21	120
H25B	924.68	1504.04	3545.37	120
H25C	1520.47	1509.16	3161.51	120
H26A	1847.34	2228.9	2849.8	108
H26B	1283.09	2747.59	2820.84	108
H26C	911.28	2255.86	2521.97	108
H27A	8968.79	4199.92	6923.7	91
H27B	9177.74	4062.26	7456.95	91
H27C	8814.25	4621.9	7293.1	91
H28A	1365.14	2833.59	4709.41	73
H28B	1215.02	3037.86	5196.37	73
H28C	983.11	2453.54	5047.74	73
H30A	5473.42	1719.62	5796.3	102
H30B	6344.14	1582.68	6152.46	102
H30C	6375.34	1644.49	5620.72	102
H31A	6449.63	3714.89	2149.18	96
H31B	6035.69	4232.46	1907.77	96
H31C	5446.8	3850.22	2144.6	96

Atom	*x*	*y*	*z*	U(eq)
H32A	3001.51	4645.5	2376.1	94
H32B	3416.2	4410.41	2865.29	94
H32C	2387.29	4509.7	2735.05	94
H34A	5164.34	4717.36	2508.85	85
H34B	6018.87	5056.49	2500.69	85
H34C	5808.82	4855.11	2977	85
H33A	7143.1	3394.02	6942.89	76
H33B	8071.5	3261.35	7250.16	76
H33C	8014.47	3462.12	6737	76
H35A	5922.17	2952.18	6298.44	106
H35B	6164.88	2451.96	6611.32	106
H35C	5254.98	2478.19	6260.35	106
H36A	7470.49	4516.93	2989.52	84
H36B	7329.06	4706.17	2469.2	84
H36C	7577.36	4117.6	2593.48	84
H38A	197.36	5072.67	3778.01	89
H38B	-767.97	5058.45	3479.85	89
H38C	47.75	5174.76	3238.83	89
H41A	2662.77	3566.75	6453.79	94
H41B	2721.67	3967.84	6051.82	94
H41C	2313.94	4144.2	6482.91	94
H42A	10042.09	5305.48	6279.68	115
H42B	10272.94	5819.57	6575.1	115
H42C	10160.35	5840.61	6029.93	115
H43A	5993.16	1608.06	3907.02	130
H43B	5974.11	1522.49	4437.6	130
H43C	5991.52	2094.79	4237.7	130
H44A	7990.55	2448.31	3705.17	84
H44B	7403.38	2956.55	3690.74	84
H44C	7081.59	2427.12	3881.13	84
H45A	2183.7	1822.17	5036.09	84
H45B	3177.44	2002.27	5184.07	84
H45C	2621.76	2178.17	4701.53	84

Atom	*x*	*y*	*z*	U(eq)
H46A	440.47	4855.13	5172.42	67
H46B	446.08	5275.19	4778.89	67
H46C	462.01	5456.92	5294.25	67
H47A	9344.2	2807.6	4665.99	103
H47B	9227.76	3029.25	4156.44	103
H47C	9217.41	2419.64	4240.54	103
H48A	3979.02	1455.19	3466.46	85
H48B	4213.27	1027.36	3857.61	85
H48C	4933.65	1205.32	3570.32	85
H49A	8083.46	5552.03	6590.35	92
H49B	8862.15	5850.83	6912.03	92
H49C	8994.59	5266.85	6764.17	92
H50A	10189.18	3655.32	5388.83	87
H50B	11046.73	3784.08	5757.49	87
H50C	10251.68	4184.2	5670.47	87
H52A	-363.68	4611.03	2718.41	80
H52B	-804.16	4072.28	2808.2	80
H52C	211.14	4095.66	2782.54	80
H54A	10059.59	4020.71	6619.29	106
H54B	11008.84	3834.93	6556.26	106
H54C	10367.19	3440.65	6743.2	106
H55A	-389.11	2190.54	2865.16	125
H55B	-113.72	2695.91	3166.28	125
H55C	-279.44	2164.28	3410.03	125
H56A	-303.07	3727.18	3719.08	90
H56B	-1159.99	4052.43	3516.95	90
H56C	-522.02	4243.27	3970.65	90
H58A	1755.45	3504.21	2608.16	122
H58B	1773.52	3440.83	2075.13	122
H58C	1491.6	3979.32	2267.21	122
H59A	2252.07	5848.01	3760.36	106
H59B	2339.01	5270.31	3584.38	106
H59C	2356.29	5745.58	3242.92	106

Atom	*x*	*y*	*z*	U(eq)
H60A	4700.21	1820.77	4767.25	80
H60B	4407.08	1259.93	4572.15	80
H60C	3752.93	1738.06	4461	80
H62A	3814.25	5844.3	5320.23	130
H62B	3761.93	6394.23	5558.12	130
H62C	3903.98	5882.42	5863.61	130
H63A	3999.31	5672.83	3149.48	228
H63B	3374.69	5197.39	3208.29	228
H63C	4358.52	5205.99	3483.65	228
H64A	7393.68	5211.06	3614.87	51
H64B	7556.29	5805.87	3748.05	51
H64C	6596.3	5567.06	3693.85	51

Table S8. Solvent mask information for 20210518_008_au24_bruker

Number	X	Y	Z	Volume	Electron count	Content
1	0.055	0.180	0.436	9.6	1.3	?
2	0.172	0.293	0.734	388.8	88.1	2 CH2Cl2
3	-0.328	0.207	0.234	388.8	89.3	2 CH2Cl2
4	-0.013	0.395	0.467	18.1	0.0	?
5	0.172	0.707	0.234	388.8	89.2	2 CH2Cl2
6	-0.013	0.605	0.967	18.1	0.0	?
7	-0.328	0.793	0.734	388.8	87.8	2 CH2Cl2
8	0.055	0.820	0.936	9.6	1.7	?
9	0.487	0.105	0.967	18.1	0.0	?
10	0.487	0.895	0.467	18.1	0.0	?
11	0.555	0.320	0.936	9.6	1.6	?
12	0.555	0.680	0.436	9.6	1.3	?