Metal Ion Independent Conductance Through Bis-Chelated Metal Complex Molecular Wires based on a Bis(diphenylphosphino)aniline Derivative

Marco F. Gatto,[a,#] Sara Sangtarash,[b,*,#] David Jago,[c] R. Tom Abram,[a] Eleanor Barrett,[a] Amit Sil,[a] George A. Koutsantonis,[c] Simon J. Higgins,[a] Craig M. Robertson,[a] Richard J. Nichols,[a] Hatef Sadeghi[b,*] & Andrea Vezzoli [a,*]

a) Department of Chemistry, University of Liverpool, Crown Street, Liverpool L69 7ZD, UK

b) Device Modelling Group, School of Engineering, University of Warwick, Coventry CV4 7AL, United Kingdom

c) School of Molecular Sciences, University of Western Australia, Perth, Western Australia 6009, Australia

#: these authors contributed equally to this work

* corresponding authors: andrea.vezzoli@liverpool.ac.uk

hatef.sadeghi@warwick.ac.uk

sara.sangtarash@warwick.ac.uk

1. NMR Spectra

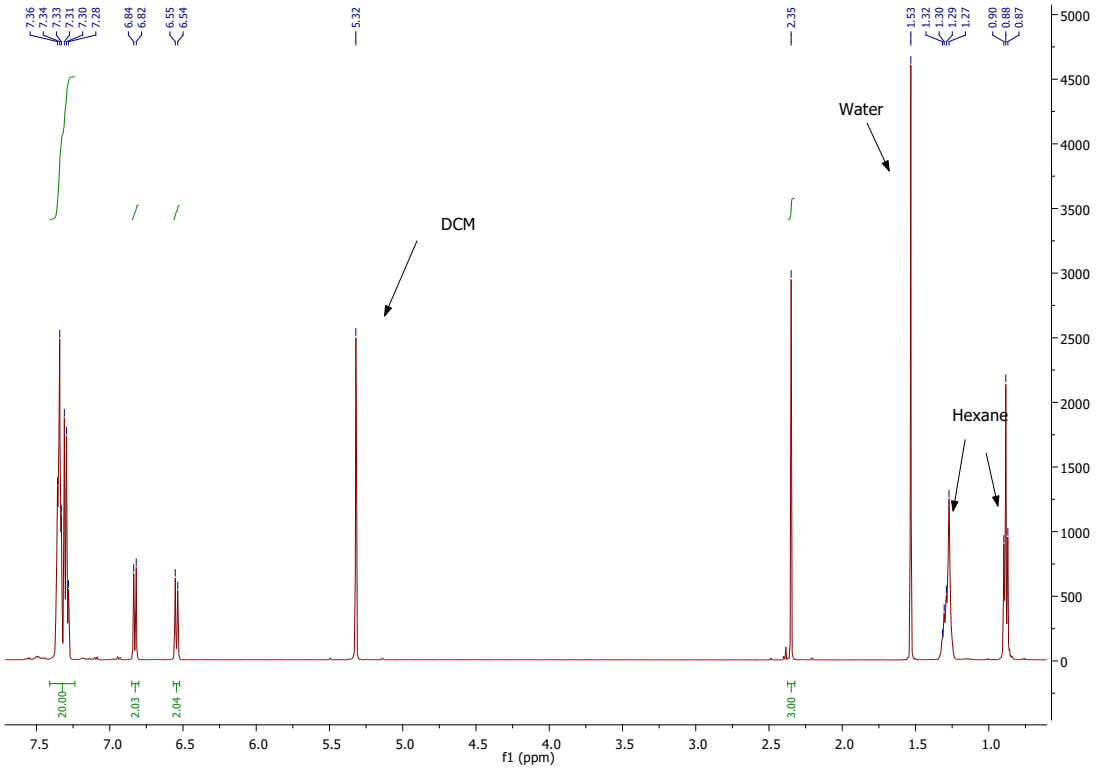

Figure S1: ^{1}H NMR (500 MHz, CD_2Cl_2) of **L**

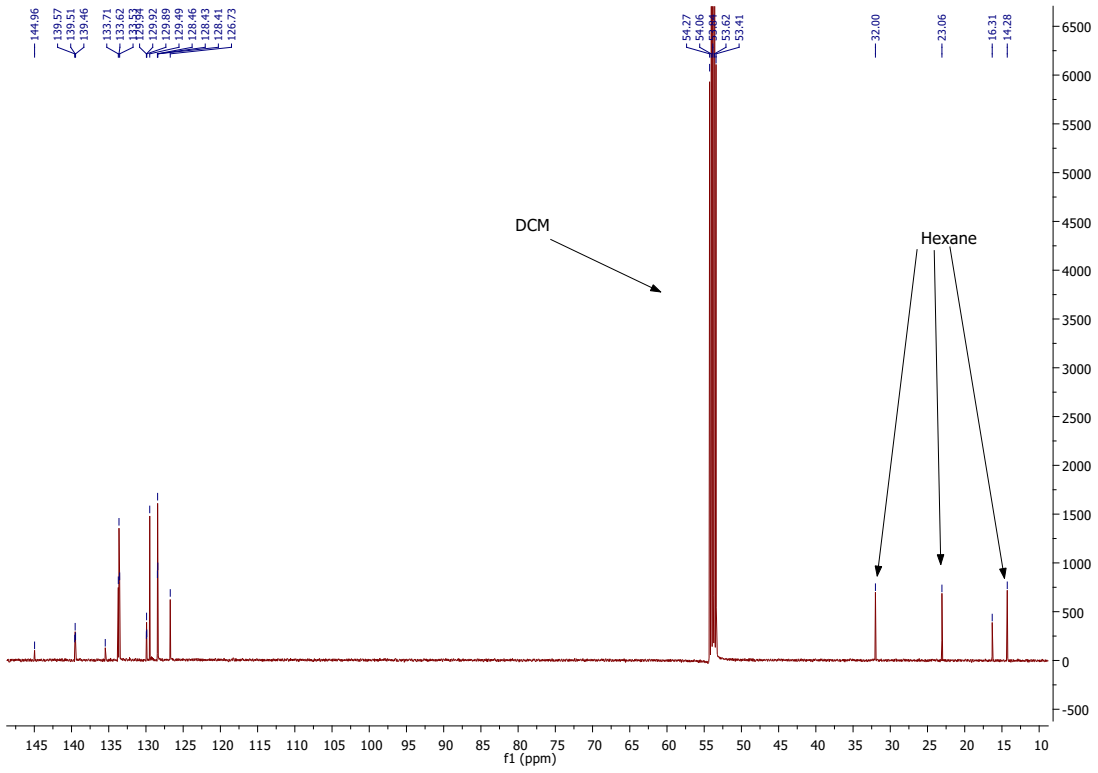

Figure S2: $^{13}C\{1H\}$ NMR (126 MHz, CD_2Cl_2) of **L**

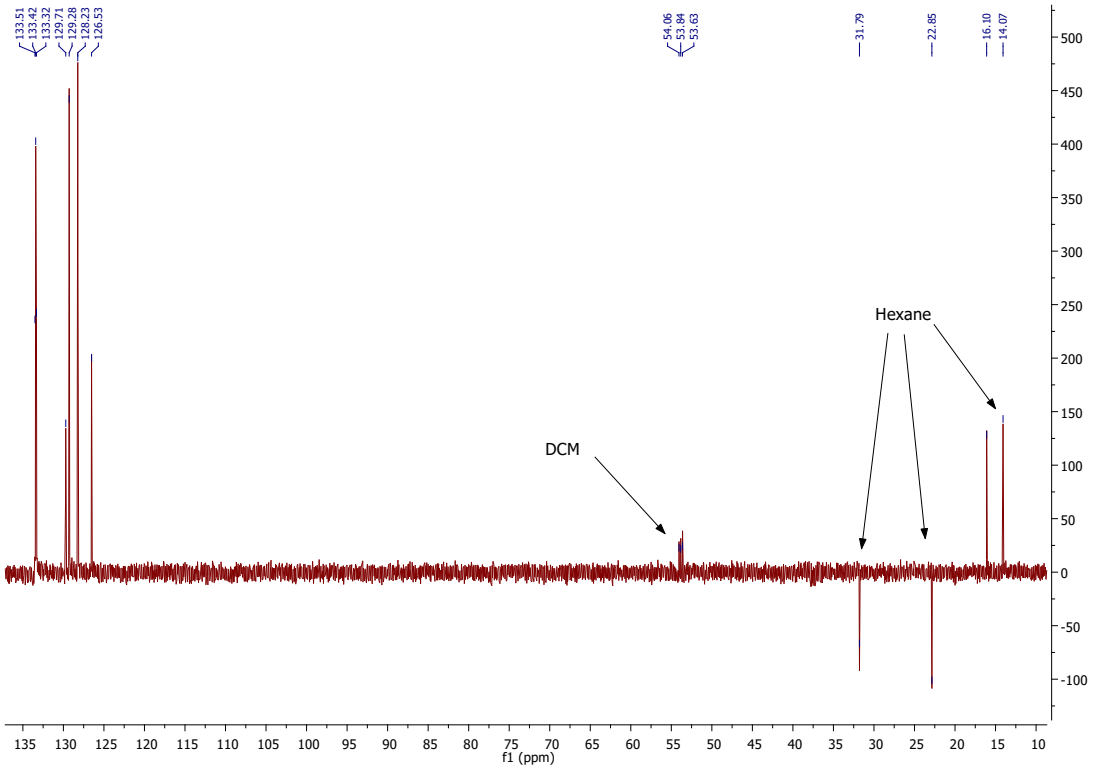

Figure S3: DEPT135 NMR (500 MHz, CD_2Cl_2) of **L**

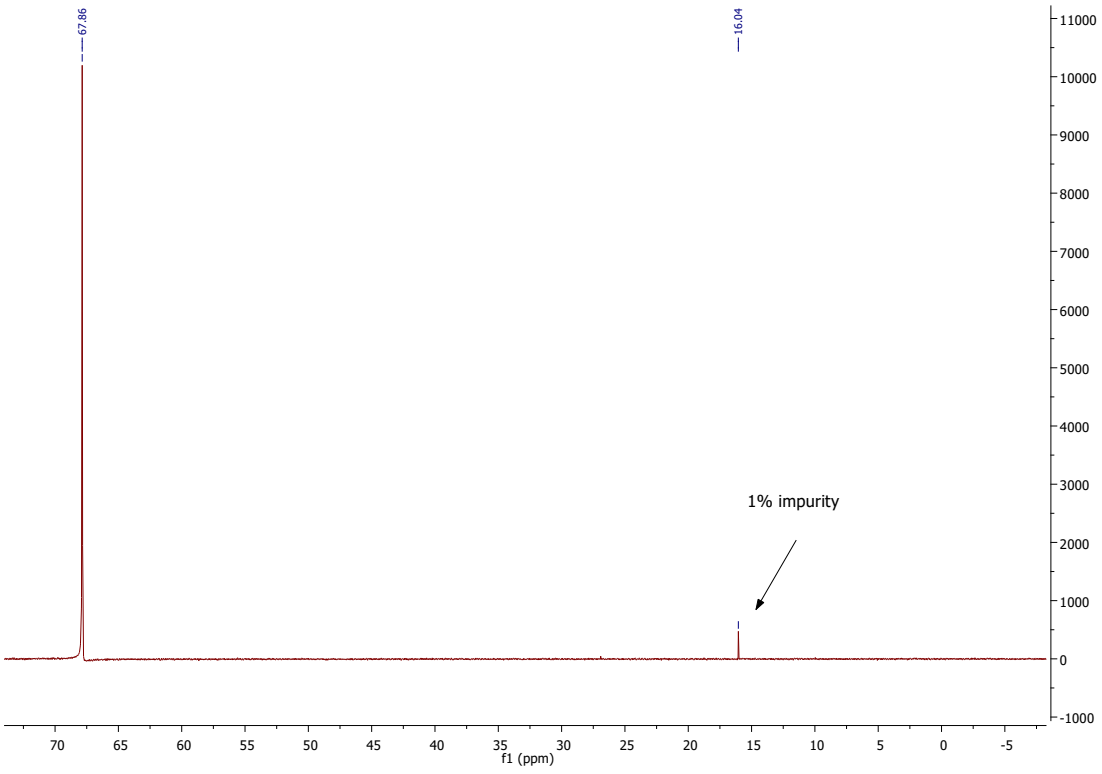

Figure S4: $^{31}P\{1H\}$ NMR (202 MHz, CD_2Cl_2) of **L**

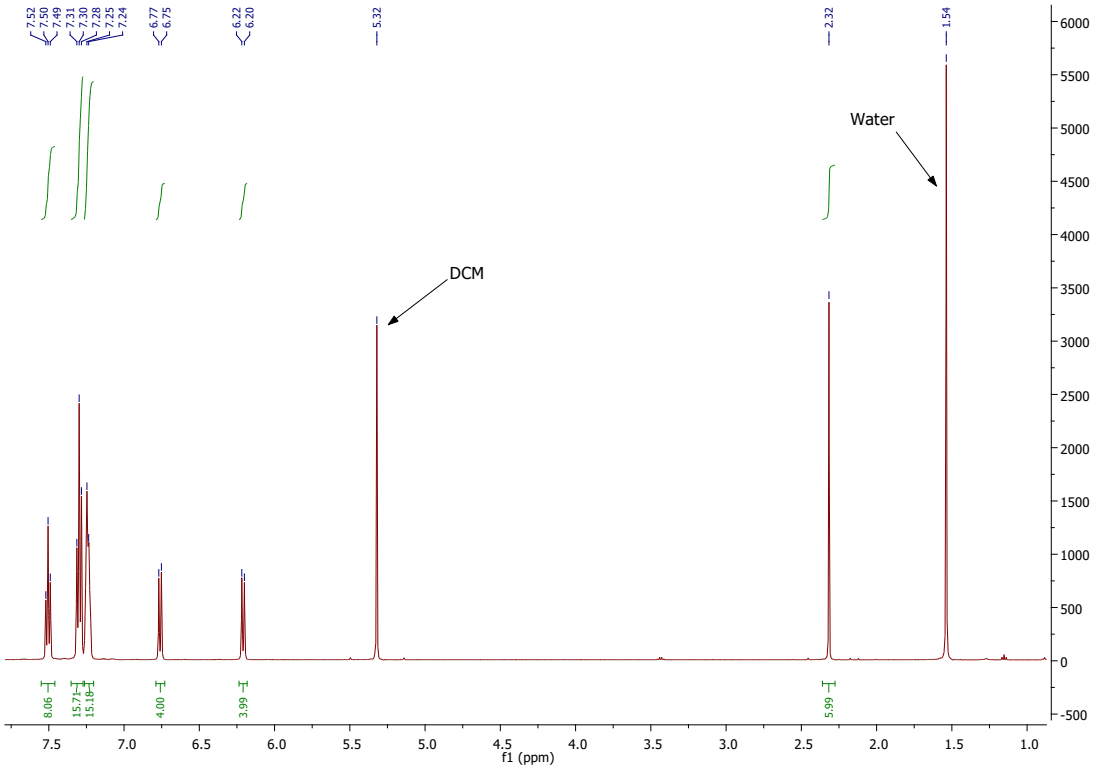

Figure S5: ^{1}H NMR (500 MHz, CD_2Cl_2) of **1**

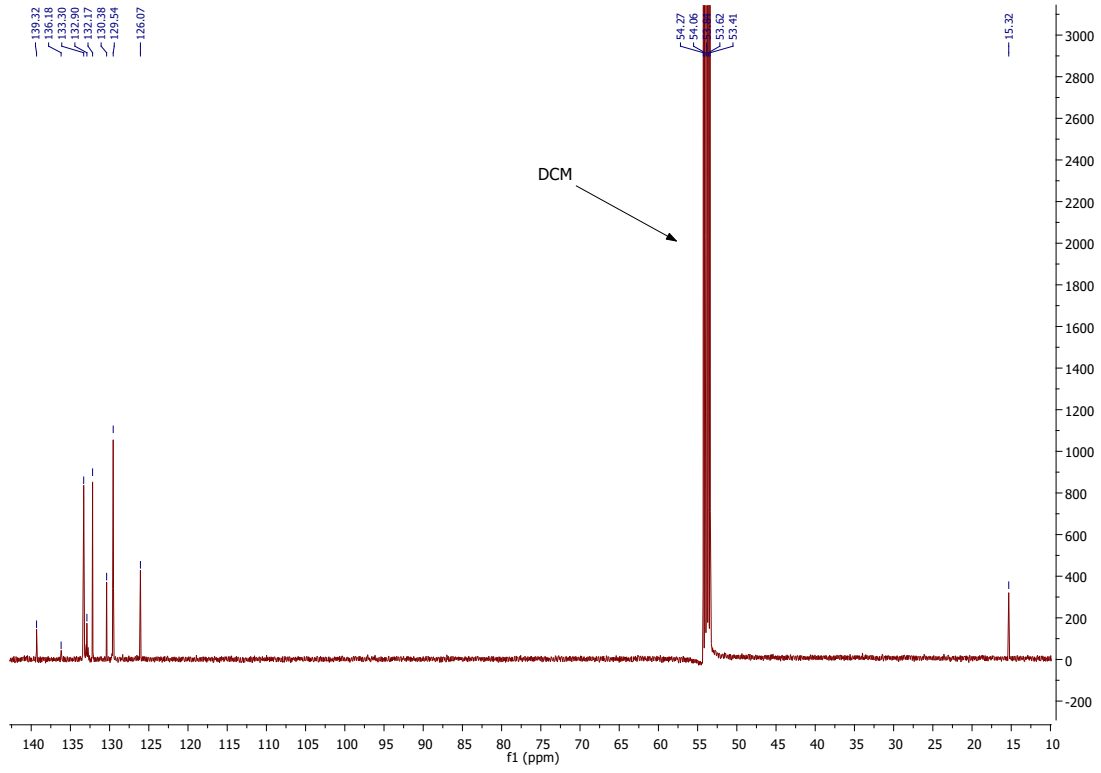

Figure S6: $^{13}C\{1H\}$ NMR (126 MHz, CD_2Cl_2) of **1**

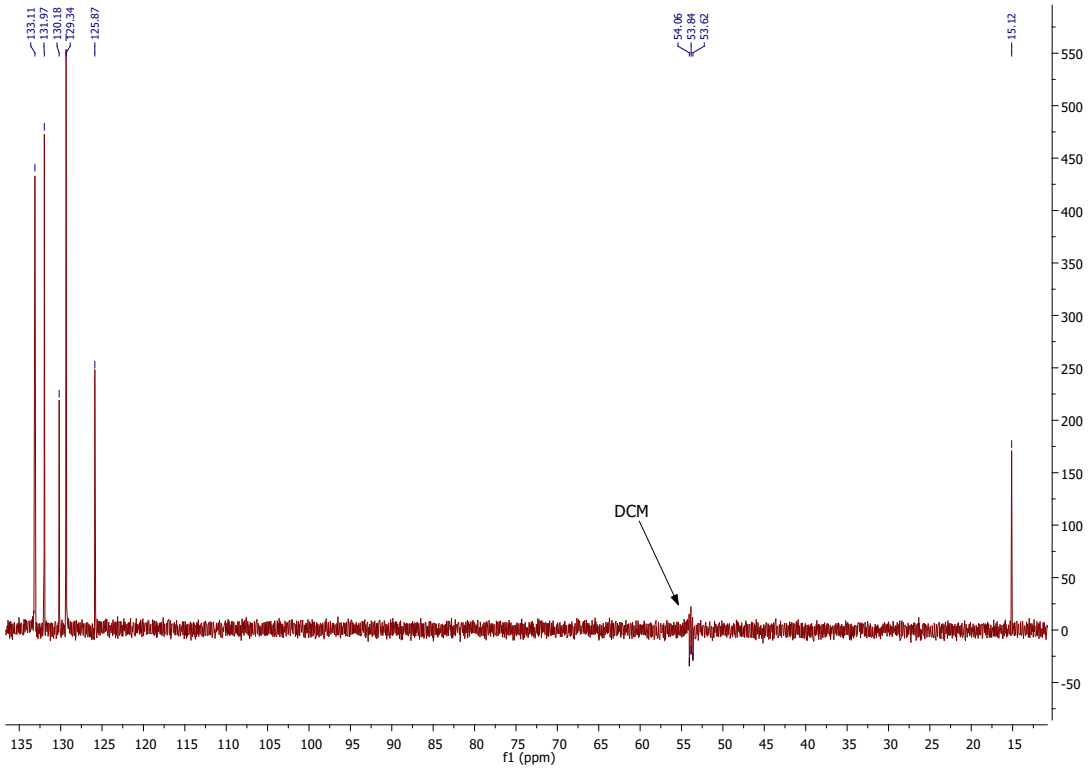

Figure S7: DEPT135 (126 MHz, CD_2Cl_2) of **1**

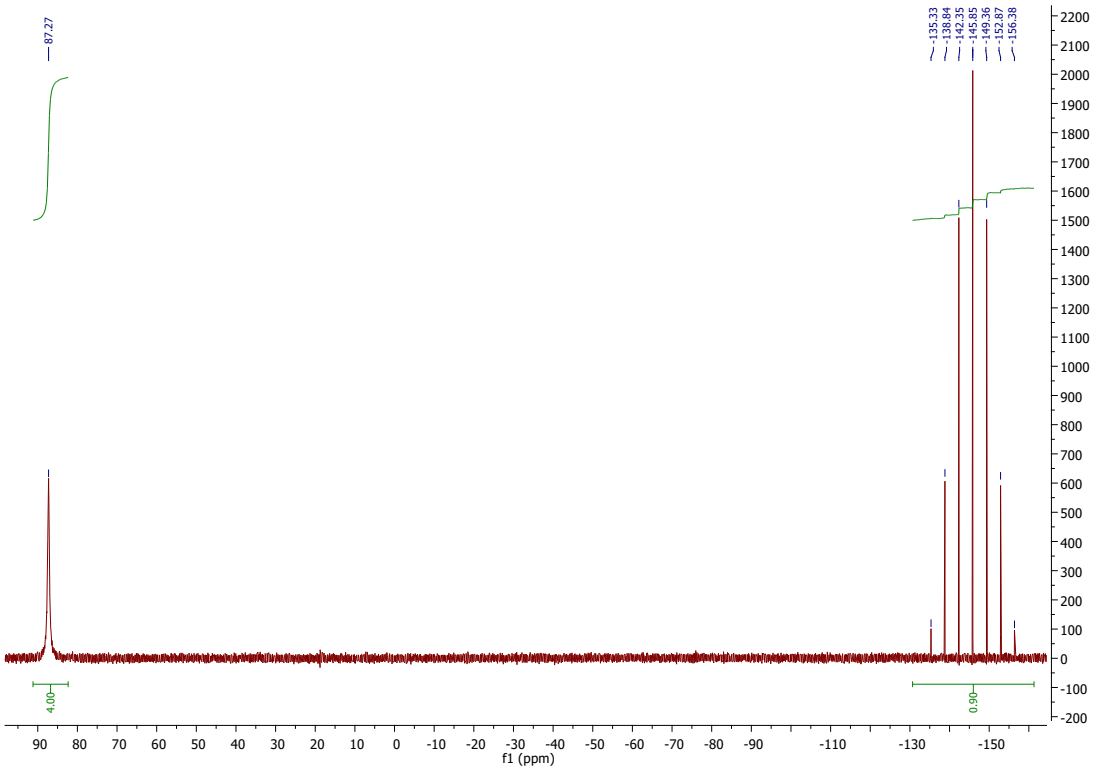

Figure S8: $^{31}P\{1H\}$ NMR (202 MHz, CD_2Cl_2) of **1**

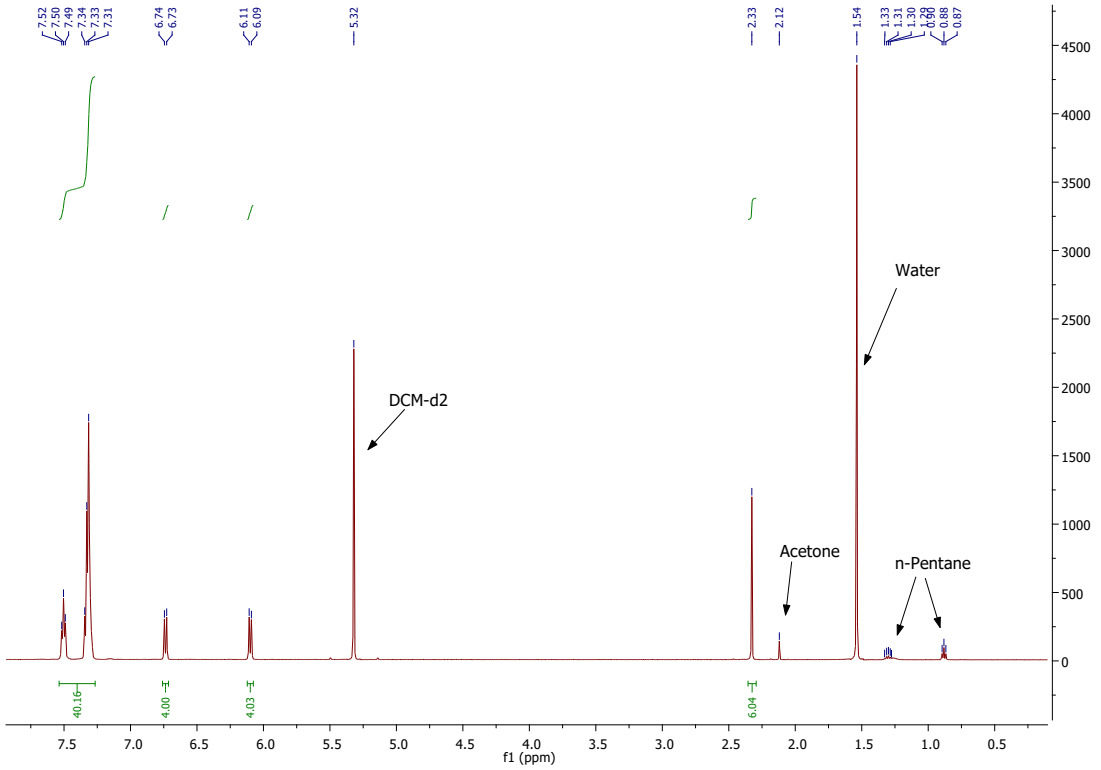

Figure S 9: ^{1}H NMR (500 MHz, CD_2Cl_2) of **2.**

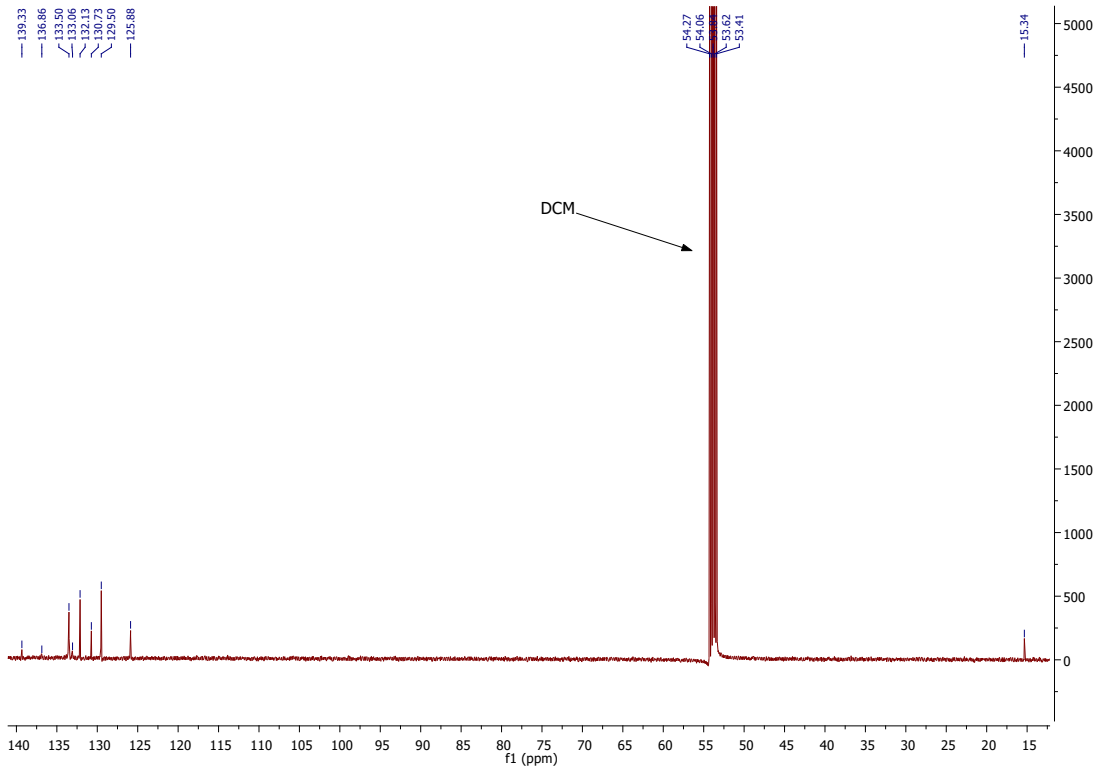

Figure S10: $^{13}C\{1H\}$ NMR (126 MHz, CD_2Cl_2) of **2**

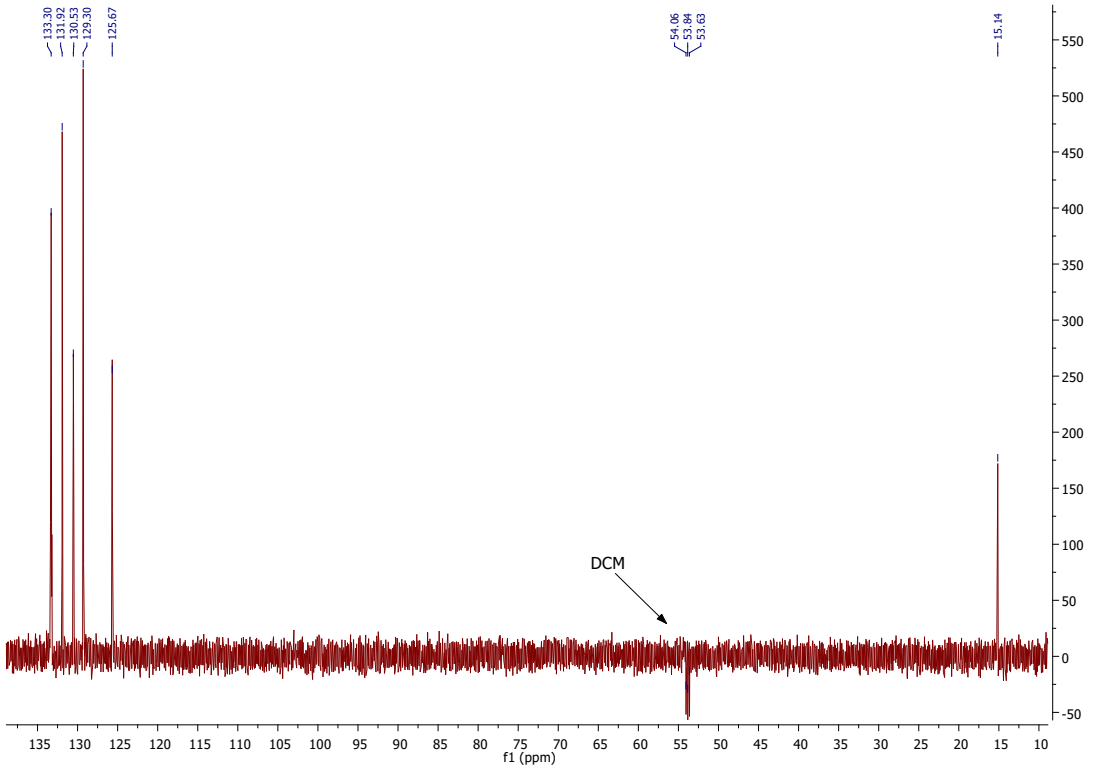

Figure S11: DEPT135 (500 MHz, CD_2Cl_2) of **2**

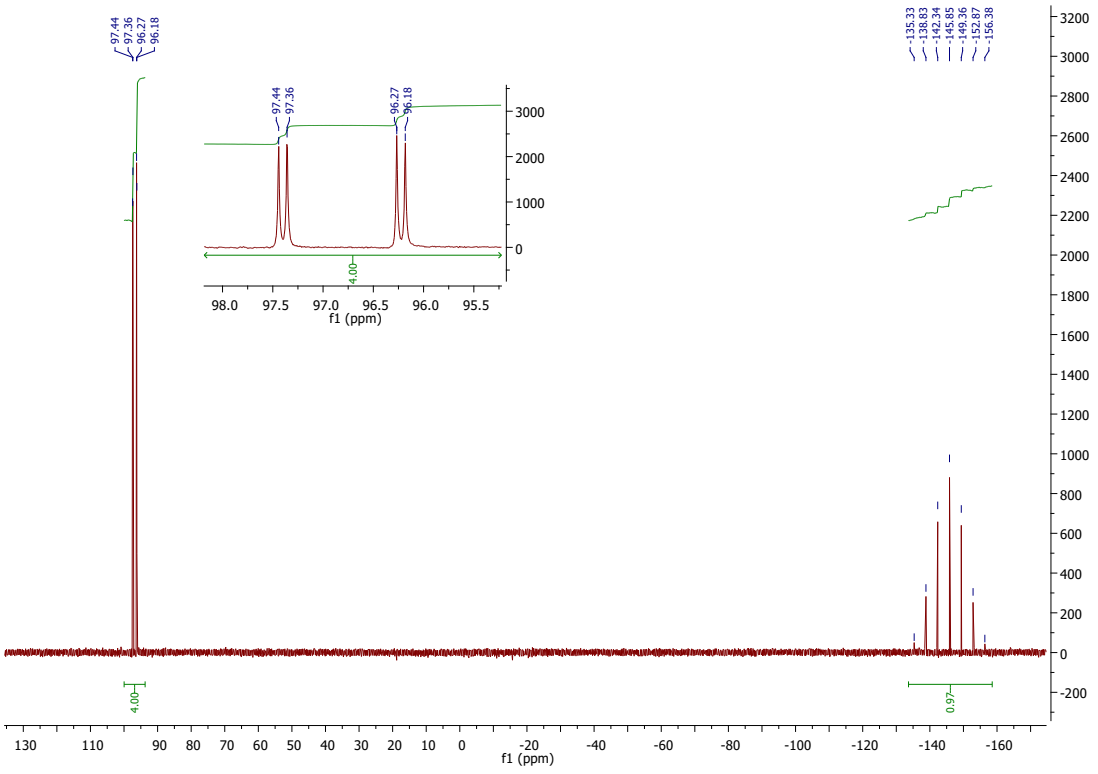

Figure S12: $^{31}P\{1H\}$ NMR (202 MHz, CD_2Cl_2) of **2**

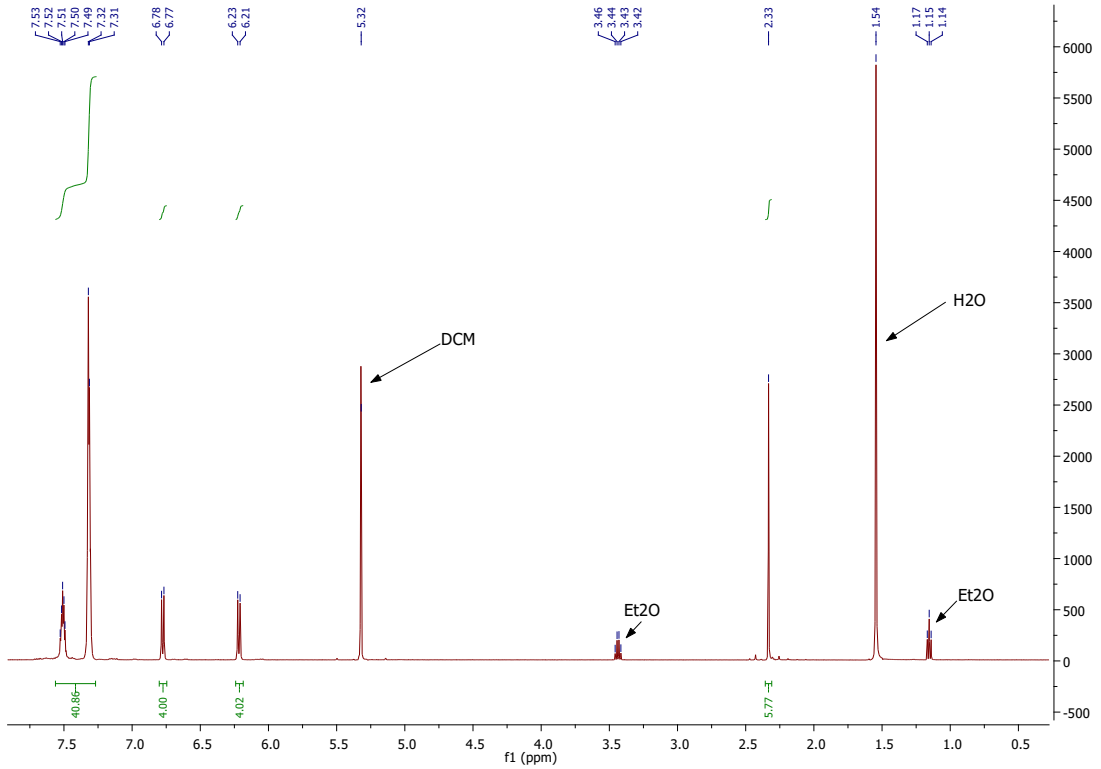

Figure S13: ^{1}H NMR (500 MHz, CD_2Cl_2) of **3**

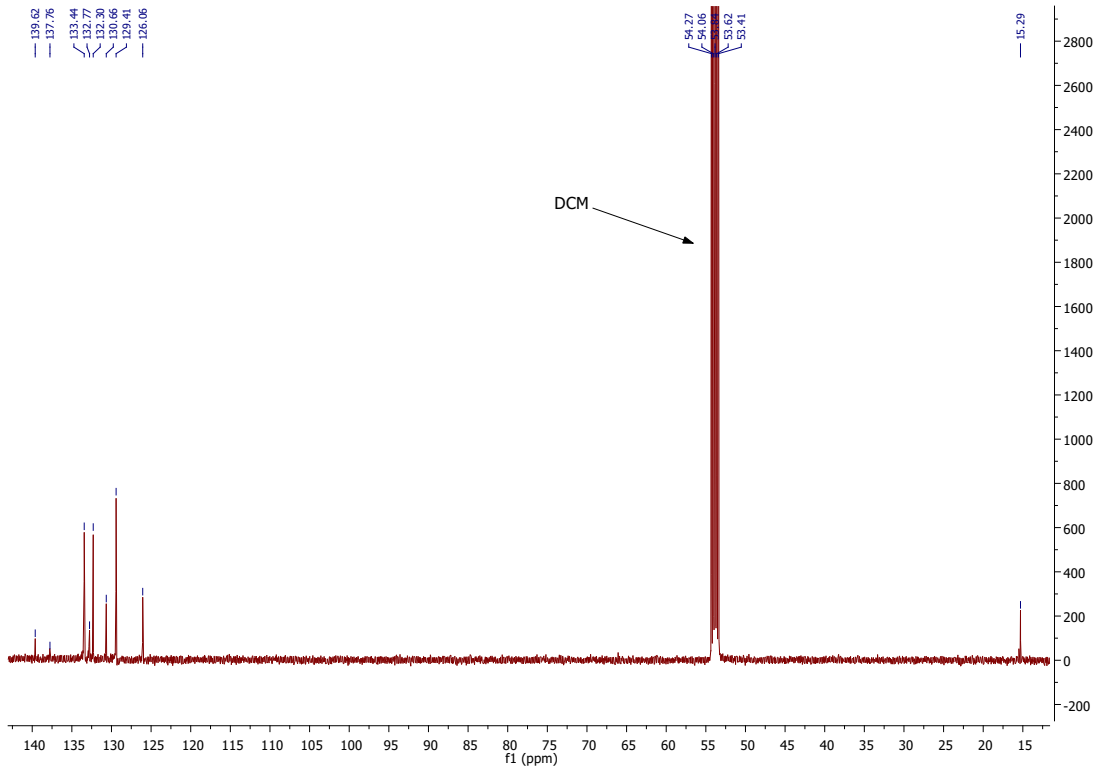

Figure S14: $^{13}C\{1H\}$ NMR (126 MHz, CD_2Cl_2) of **3**

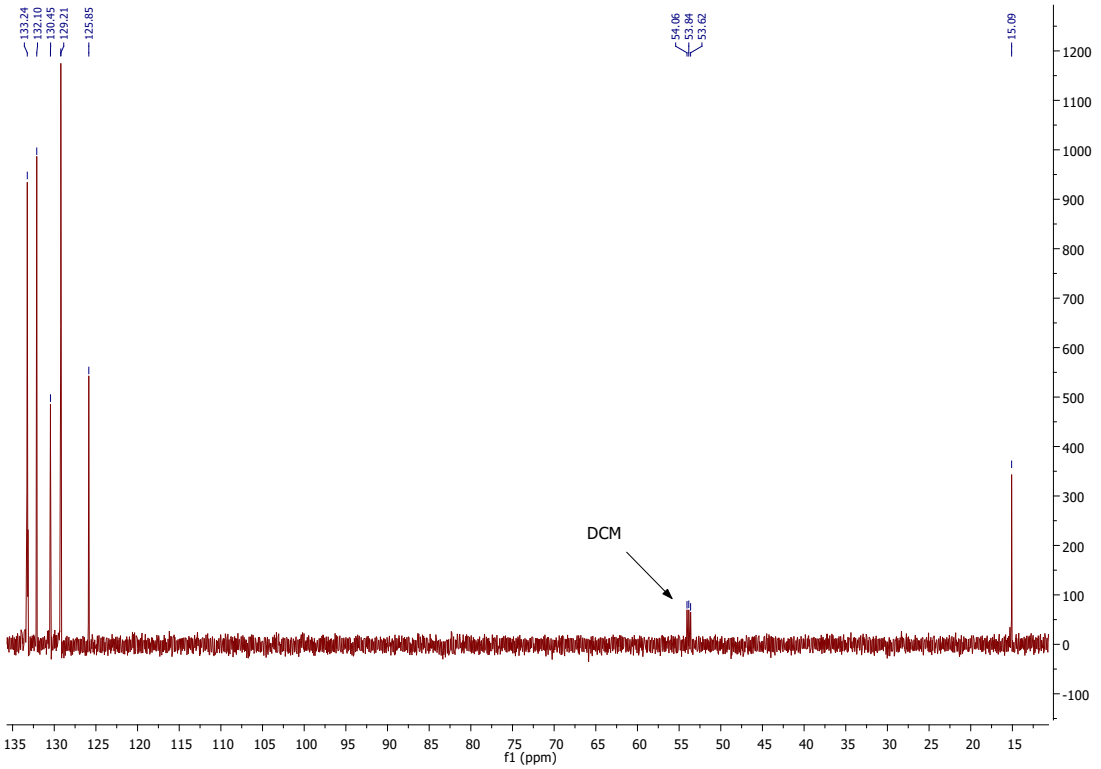

Figure S15: DEPT135 (126 MHz, CD_2Cl_2) of **3**

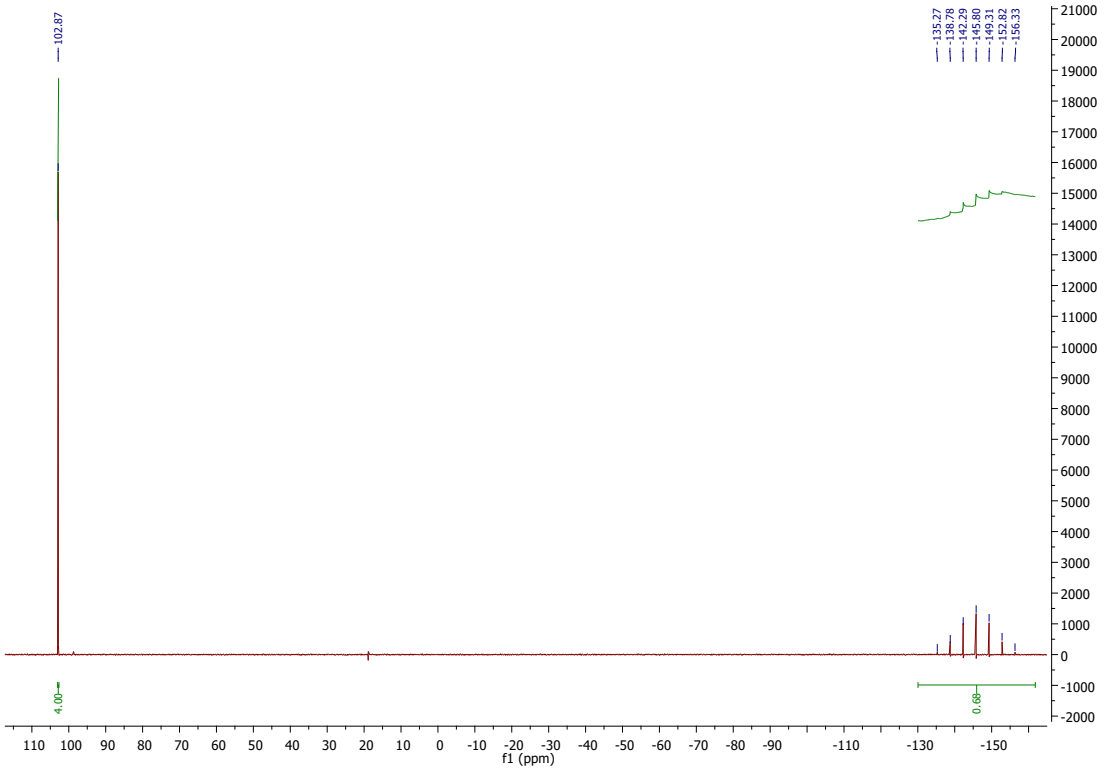

Figure S16: $^{31}P\{1H\}$ NMR (202 MHz, CD_2Cl_2) of 3

2. Details on STMBJ measurements

We used a modified Keysight 5500 scanning tunnelling microscope (Figure S17: Schematics of the modified Keysight 5500 STM used in this study), equipped with a Femto DLPCA-200 current amplifier. Piezo voltage and tip bias are imposed by an Arbitrary Wavefunction Generator (AWG, Keysight 33522B), and signals are recorded with a National Instrument PXI system (24-bit PXI-4464 DAQ, PXIe-1062Q chassis, PXIe-PCIe8381 interface). The *Z* piezo voltage signal is fed directly into the STM controller, that has an in-built voltage amplifier to convert the $\pm 10\,V$ signal of the AWG to the $\pm 215\,V$ that drive the *Z* piezoelectric transducer. In this study, we employed a $100\,k\Omega$ or $200\,k\Omega$ resistor after the function generator, to reduce the bias applied (0.3 V or 0.5 V) to junctions of conductance $> 0.1\,G_0$. As discussed in our recent publication,[1] the resistor prevents overload of the amplifier and causes an almost complete junction bias drop at values of conductance $> G_0$, extending the measurement window to ~8 orders of magnitude (from $\cong 10^2 G_0$ to $\cong 10^{-6} G_0$) and protecting the fragile Au atomic contact from electromigration.

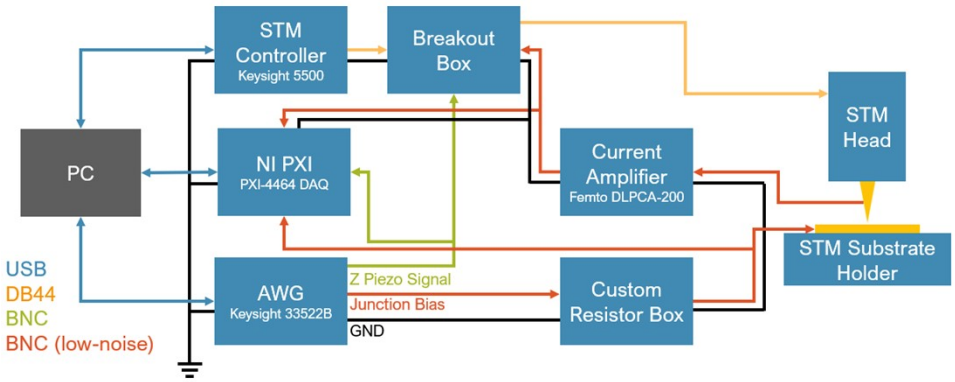

Figure S17: Schematics of the modified Keysight 5500 STM used in this study

The STMBJ experiments in this study have been performed using an Au tip cut from a spool of Au wire (99.998%, ThermoFisher Scientific PREMION), and substrates are prepared by e-beam evaporation (Korvustech HEX Tau4) of ~100 nm of Au on freshly cleaved mica (muscovite, Agar Scientific). Substrates were briefly flame-annealed with a butane torch before use. Experiments were all performed after deposition of the above salts from an about 0.1 mM of their anisole solution on to the gold layer for about 2 hrs directly into the liquid cell, then the solvent was withdrawn by a syringe and the liquid cell was washed three times by mesitylene. All the measurements were conducted in mesitylene (1,3,5-trimethylbenzene 98+%, TCI UK). Further information is available in our previous publications.[2,3]

2.1 STMBJ Measurements

Bespoke software written in LabVIEW controls the instrument and acquires data. We continuously record the signal applied to the piezoelectric transducer V_Z, the junction bias V_{BIAS} and the output of the Femto amplifier V_{OUT}, at a rate of $20\ kSa/s$ and a resolution of 24 bits. The current I is calculated from V_{OUT} using the amplification factor ($10^6\ V/A$ in this study) and the junction bias is then calculated using Ohm's law $G = I/V_{BIAS}$ in units of G_0. The tip displacement is calculated from the value of V_Z using the amplification factor of the STM controller electronics (10:215 ratio) and the calibration against Au(111) atomic step height (currently $19.1\ \text{Å}/V$). A trigger/gate function cuts the continuous stream of data into single traces representative of a single cycle of tip approach and withdrawal. Each trace is then checked by an automated algorithm, that ensures that a clean metallic junction of $G > 5G_0$ is fabricated as the tip is crashed into the substrate, and that the current decays below the noise level of the instrument (~ 50 pA) at the end of the *Z* ramp. The piezo is moved at a constant speed of $10\ nm/s$ in this study. All data that satisfies the conditions described earlier are then used without further selection, and compiled into histograms, density plots and correlogram as presented in the manuscript and here in the SI.

2,2 Data and Software availability

Raw data and LabVIEW Vis used for its processing can be accessed free of charge on the University of Liverpool Data Catalogue, at the DOI specified in the Data Availability section of the manuscript. Executable versions of the Vis (*i.e.* not requiring a LabVIEW license to run) are available from the authors upon request. The runtime required to run the executables can be downloaded freely from the National Instruments website.†

† https://www.ni.com [retrieved 17/07/2023]

3. Additional STMBJ Data

In addition to the plots presented in the manuscript, we show here histograms and 2D density maps (conductance *vs* electrode separation *vs* counts) for **1 − 3** obtained applying a bias of 0.5 V, along with relevant experimental details in each figure caption.

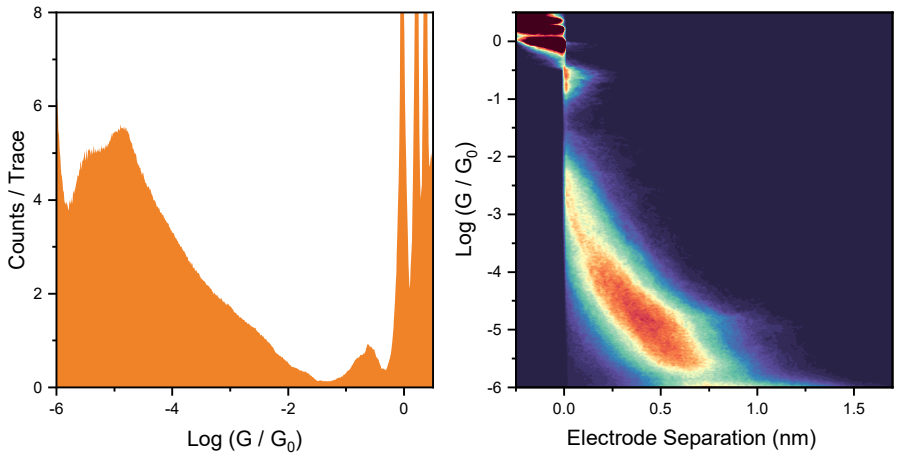

Figure S18: Conductance histogram and 2D map for **1**. Data acquired at $500\ mV$, $10\ nm\ s^{-1}$ in mesitylene after deposition on gold layer as explained above. Plots compiled from 7202 individual STMBJ traces. 100 bins per conductance decade, 100 bins per nm.

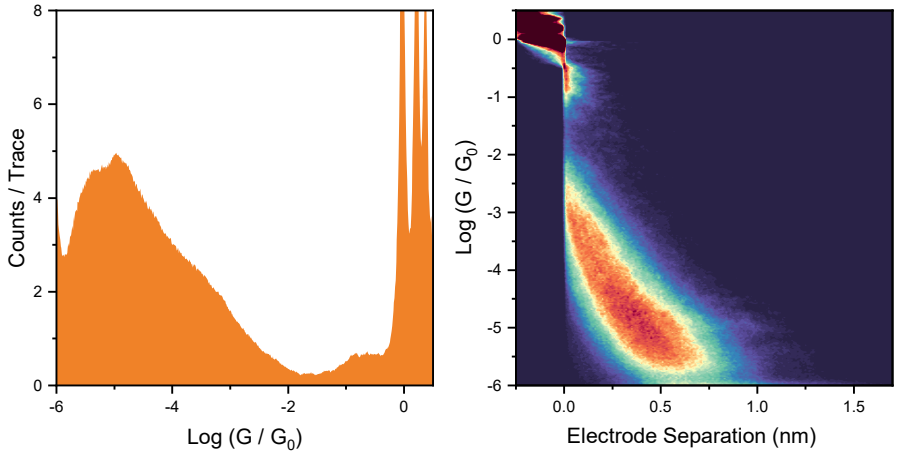

Figure S19: Conductance histogram and 2D map for **2**. Data acquired at $500\ mV$, $10\ nm\ s^{-1}$ in mesitylene after deposition on gold layer as explained above. Plots compiled from 3941 individual STMBJ traces. 100 bins per conductance decade, 100 bins per nm.

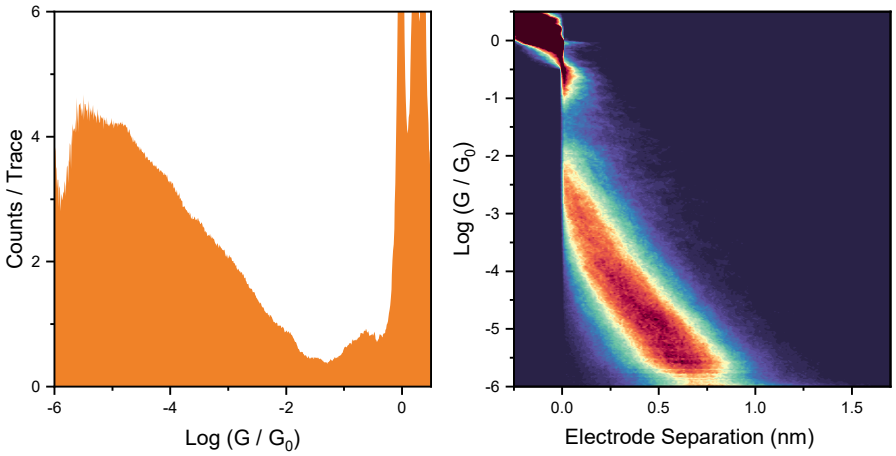

Figure S20: Conductance histogram and 2D map for **3**. Data acquired at $500\ mV$, $10\ nm\ s^{-1}$ in mesitylene after deposition on gold layer as explained above. Plots compiled from 5487 individual STMBJ traces. 100 bins per conductance decade, 100 bins per nm.

3.2 Additional data at lower tip-substrate bias

We also show here data acquired at 0.3 V bias, where the higher noise floor prevents clear observation of the histogram peak, but similar conductance behaviour can be observed.

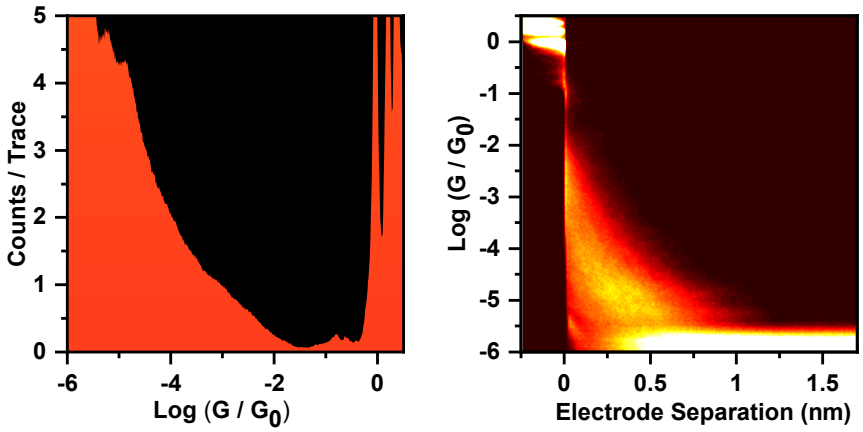

Figure S21: Conductance histogram and 2D map for **1**. Data acquired at $300\ mV$, $10\ nm\ s^{-1}$ in mesitylene after deposition on gold layer as explained above. Plots compiled from 5409 individual STMBJ traces. 100 bins per conductance decade, 100 bins per nm.

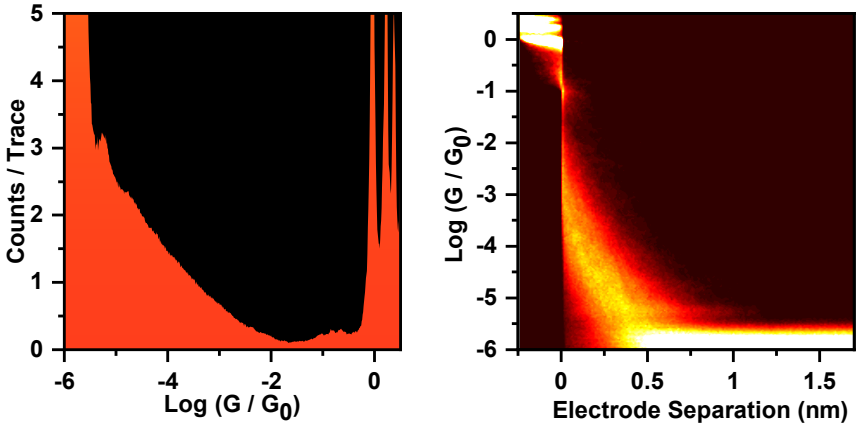

Figure S22: Conductance histogram and 2D map for **2**. Data acquired at $300\ mV$, $10\ nm\ s^{-1}$ in mesitylene after deposition on gold layer as explained above. Plots compiled from 3727 individual STMBJ traces. 100 bins per conductance decade, 100 bins per nm.

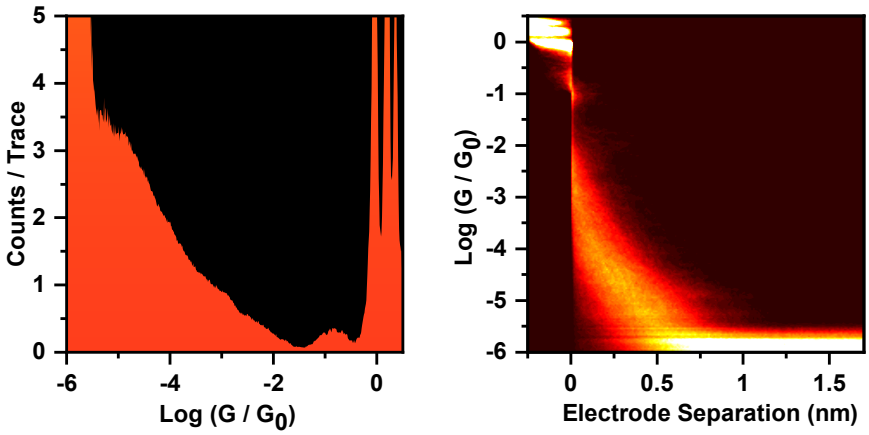

Figure S23: Conductance histogram and 2D map for **3**. Data acquired at $300\ mV$, $10\ nm\ s^{-1}$ in mesitylene after deposition on gold layer as explained above. Plots compiled from 4037 individual STMBJ traces. 100 bins per conductance decade, 100 bins per nm.

4. Additional Raman Spectroscopy and SERS Data

In addition to the data presented in the main manuscript on **1**, we show here the full spectra for all compounds, either acquired in their powder form or adsorbed on Au nanoparticles in SERS experiments.

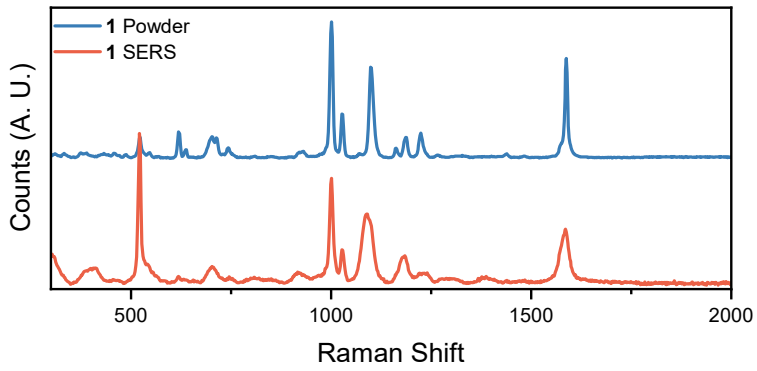

Figure S24: Comparison between powder Raman (blue) and SERS (red) spectra for **1**.

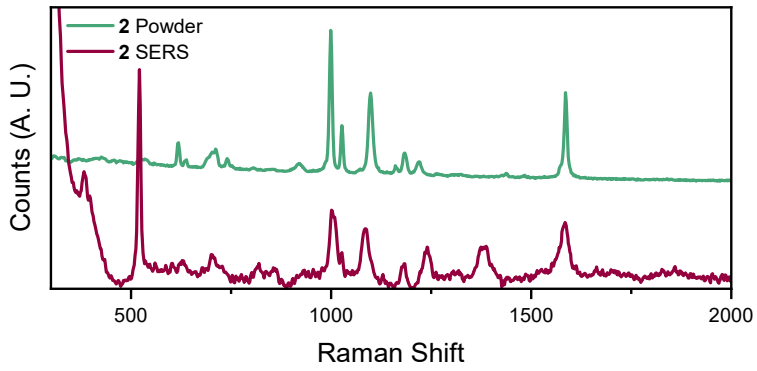

Figure S 25: Comparison between powder Raman (teal) and SERS (brown) spectra for **2**.

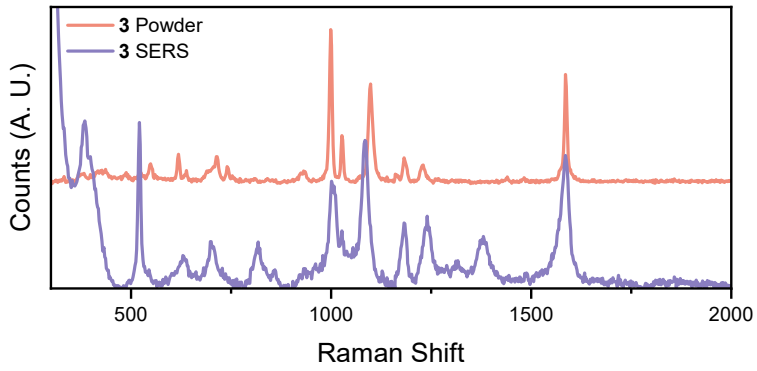

Figure S26: Comparison between powder Raman (teal) and SERS (brown) spectra for **2**.

It can be seen here that many of the arguments raised for **1** in the main paper can be made here for the other two compounds in the series. The signals relative to the ancillary phenyl ring modes (~1600 cm^{-1}) are broadened in the SERS spectra due to interaction with Au, and those relative to the thioanisole are either shifted (~1100 cm^{-1}) or broadened/merged (~700 cm^{-1}), supporting strong Au-S interactions.

5. XRD Details, Structures and Crystallographic Parameters

5.1 Details and Tables for 1

Single crystals of $C_{62}H_{54}CuF_6N_2S_7P_{0.5}$ [final40s] was submitted for single crystal determination. A suitable crystal was selected and mounted on a MiTeGen tip using Parabol oil and placed on a Bruker APEX-II CCD diffractometer. The crystal was kept at 199.99 K during data collection. Using Olex2,[4] the structure was solved with the XT[5] structure solution program using Intrinsic Phasing and refined with the XL[6] refinement package using Least Squares minimisation. PLATON squeeze algorithm was used to remove void space electron density from highly disordered DCM solvent molecules. Approximately 7 CH_2Cl_2 molecules in the unit cell were removed.

Crystal Data for $C_{62}H_{54}CuF_6N_2S_7P_{0.5}$ (M =1244.51 g/mol): monoclinic, space group P2/c (no. 13), a = 12.2541(13) Å, b = 13.7569(15) Å, c = 20.607(2) Å, β = 107.028(4)°, V = 3321.6(6) Å^3, Z = 2, T = 199.99 K, μ(MoKα) = 0.614 mm^{-1}, *Dcalc* = 1.244 g/cm^3, 63228 reflections measured (4.566° ≤ 2Θ ≤ 53.484°), 6934 unique (R_{int} = 0.1389, R_{sigma} = 0.0599) which were used in all calculations. The final R_1 was 0.1184 (I > 2σ(I)) and wR_2 was 0.2443 (all data).

Table 1 Crystal data and structure refinement for final40s.

Identification code	final40s
Empirical formula	$C_{62}H_{54}CuF_6N_2S_7P_{0.5}$
Formula weight	1244.51
Temperature/K	199.99
Crystal system	monoclinic
Space group	P2/c
a/Å	12.2541(13)
b/Å	13.7569(15)
c/Å	20.607(2)
α/°	90
β/°	107.028(4)
γ/°	90
Volume/Å^3	3321.6(6)
Z	2
ρ_{calc}g/cm^3	1.244
μ/mm^{-1}	0.614
F(000)	1285.0
Crystal size/mm^3	0.32 × 0.02 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.566 to 53.484
Index ranges	-15 ≤ h ≤ 15, -17 ≤ k ≤ 17, -25 ≤ l ≤ 25
Reflections collected	63228
Independent reflections	6934 [R_{int} = 0.1389, R_{sigma} = 0.0599]
Data/restraints/parameters	6934/0/354
Goodness-of-fit on F^2	1.120
Final R indexes [I>=2σ (I)]	R_1 = 0.1184, wR_2 = 0.2396
Final R indexes [all data]	R_1 = 0.1286, wR_2 = 0.2443
Largest diff. peak/hole / e Å^{-3}	1.16/-0.98

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for final40s. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu(01)	5000	7467.3(8)	7500	21.6(3)
P(2)	6432.7(14)	8047.3(12)	7107.8(8)	22.2(4)
P(1)	4937.2(14)	6579.3(12)	6545.8(8)	20.3(4)

Table 2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for final40s. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P(004)	10000	6041(2)	2500	43.6(7)
S(005)	8527(2)	6449(2)	4367.5(11)	54.9(7)
N(007)	6163(5)	7146(4)	6502(3)	22.5(11)
C(008)	3840(5)	6736(5)	5745(3)	22.4(13)
C(009)	6154(6)	4994(5)	7194(3)	27.5(14)
C(00A)	4646(6)	4583(5)	6194(3)	25.3(14)
C(00B)	6406(6)	4037(5)	7337(3)	32.5(16)
C(00C)	6746(5)	6967(5)	5997(3)	25.4(14)
C(00D)	7908(5)	7918(5)	7620(3)	25.4(14)
C(00E)	5273(5)	5296(4)	6619(3)	19.8(13)
C(00F)	6367(6)	9207(5)	6665(4)	29.7(15)
F(00G)	10930(8)	6832(6)	2854(4)	113(3)
C(00H)	3918(7)	6423(5)	5112(3)	32.4(16)
C(00I)	5774(7)	3327(6)	6901(4)	37.5(18)
C(00J)	8469(6)	7027(5)	7702(3)	27.8(14)
C(00K)	7812(6)	6609(6)	4992(4)	35.4(18)
C(00L)	6698(6)	7664(6)	5485(3)	30.1(15)
C(00M)	7323(6)	6112(5)	5993(3)	28.7(15)
C(00N)	8428(7)	8682(6)	8037(5)	44(2)
C(00O)	2853(6)	7195(6)	5772(4)	40.0(19)
C(00P)	4888(7)	3599(5)	6338(4)	33.9(17)
C(00Q)	10029(7)	7697(6)	8573(4)	44(2)
C(00R)	7247(6)	7471(6)	4998(3)	32.7(16)
C(00S)	7873(7)	5921(6)	5503(4)	34.8(17)
C(00T)	3024(7)	6559(6)	4533(4)	36.5(18)
C(00U)	9502(7)	6911(6)	8171(4)	37.2(17)
C(00V)	7310(9)	9621(7)	6530(5)	56(2)
C(00W)	2038(7)	6978(7)	4577(4)	46(2)
C(00X)	9458(8)	8552(7)	8497(5)	54(2)
F(00Y)	9102(6)	5260(5)	2190(7)	152(5)
C(010)	1947(8)	7315(8)	5186(4)	54(2)
C(011)	5349(9)	9652(7)	6437(5)	57(2)
F(012)	9547(9)	6141(11)	3114(4)	174(6)
C(013)	8597(9)	5149(9)	4284(5)	71(3)
C(014)	6149(13)	10924(8)	5936(7)	87(4)
C(015)	7165(11)	10499(8)	6153(6)	80(4)
C(016)	5180(11)	10507(8)	6051(7)	87(4)

Table 3 Anisotropic Displacement Parameters (Å²×10³) for final40s. 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}
Cu(01)	22.1(6)	25.5(6)	16.9(5)	0	5.4(4)	0
P(2)	21.0(8)	24.4(8)	20.5(8)	0.6(7)	4.8(6)	-1.2(7)
P(1)	18.9(8)	25.6(8)	15.3(7)	1.1(6)	3.4(6)	-2.1(6)
P(004)	50.3(19)	46.5(18)	41.8(17)	0	25.7(15)	0
S(005)	58.4(14)	81.8(17)	36.6(11)	-8.1(11)	32.6(11)	-23.3(13)
N(007)	25(3)	23(3)	21(3)	-3(2)	8(2)	-3(2)
C(008)	21(3)	26(3)	15(3)	1(2)	-3(2)	-3(3)
C(009)	30(4)	29(3)	22(3)	-1(3)	6(3)	-5(3)
C(00A)	26(3)	29(3)	18(3)	-3(3)	3(3)	-1(3)
C(00B)	36(4)	39(4)	21(3)	12(3)	7(3)	7(3)
C(00C)	21(3)	40(4)	13(3)	-1(3)	1(2)	-7(3)
C(00D)	12(3)	39(4)	19(3)	0(3)	-5(2)	3(3)
C(00E)	26(3)	20(3)	17(3)	-3(2)	13(3)	-4(2)
C(00F)	37(4)	19(3)	31(4)	10(3)	6(3)	-2(3)
F(00G)	158(8)	83(5)	81(5)	-17(4)	6(5)	-31(5)
C(00H)	47(4)	32(4)	18(3)	-2(3)	11(3)	-5(3)
C(00I)	51(5)	28(4)	37(4)	0(3)	19(4)	10(3)
C(00J)	22(3)	37(4)	23(3)	-3(3)	3(3)	1(3)

Table 3 Anisotropic Displacement Parameters (Å²×10³) for final40s. The Anisotropic displacement factor exponent takes the form: -2π²[h²a*²U₁₁+2hka*b*U₁₂+…].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
$C^{(00K)}$	22(4)	57(5)	26(4)	-1(3)	6(3)	-21(3)
$C^{(00L)}$	24(3)	41(4)	22(3)	3(3)	2(3)	1(3)
$C^{(00M)}$	39(4)	25(3)	27(3)	0(3)	19(3)	-12(3)
$C^{(00N)}$	37(4)	26(4)	63(6)	-5(4)	2(4)	-1(3)
$C^{(00O)}$	32(4)	54(5)	29(4)	-10(4)	0(3)	5(4)
$C^{(00P)}$	44(4)	30(4)	29(4)	-9(3)	11(3)	-4(3)
$C^{(00Q)}$	29(4)	53(5)	41(4)	-1(4)	-3(3)	3(4)
$C^{(00R)}$	27(4)	51(4)	20(3)	3(3)	7(3)	-8(3)
$C^{(00S)}$	37(4)	40(4)	33(4)	-7(3)	18(3)	-14(3)
$C^{(00T)}$	43(5)	40(4)	18(3)	1(3)	-3(3)	-10(3)
$C^{(00U)}$	38(4)	40(4)	37(4)	5(3)	17(3)	10(3)
$C^{(00V)}$	59(6)	48(5)	67(6)	23(5)	26(5)	-5(4)
$C^{(00W)}$	39(5)	60(5)	27(4)	6(4)	-9(3)	11(4)
$C^{(00X)}$	46(5)	38(5)	62(6)	-11(4)	-10(4)	-3(4)
$F^{(00Y)}$	43(4)	61(5)	315(14)	-39(7)	-4(6)	-12(3)
$C^{(010)}$	35(5)	76(7)	43(5)	3(5)	-2(4)	20(5)
$C^{(011)}$	54(6)	41(5)	74(7)	12(5)	18(5)	10(4)
$F^{(012)}$	159(9)	309(16)	81(6)	13(8)	78(6)	83(10)
$C^{(013)}$	61(7)	111(10)	51(6)	-13(6)	34(5)	10(6)
$C^{(014)}$	130(12)	40(6)	89(9)	33(6)	29(8)	-1(7)
$C^{(015)}$	85(9)	64(7)	96(9)	50(7)	33(7)	-15(6)
$C^{(016)}$	82(8)	56(7)	118(11)	56(7)	24(8)	19(6)

Table 4 Bond Lengths for final40s.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
$Cu^{(01)}$	$P^{(2)1}$	2.2809(17)	$C^{(00B)}$	$C^{(00I)}$	1.397(11)
$Cu^{(01)}$	$P^{(2)}$	2.2810(17)	$C^{(00C)}$	$C^{(00L)}$	1.414(9)
$Cu^{(01)}$	$P^{(1)}$	2.2969(17)	$C^{(00C)}$	$C^{(00M)}$	1.374(10)
$Cu^{(01)}$	$P^{(1)1}$	2.2970(17)	$C^{(00D)}$	$C^{(00J)}$	1.391(10)
$P^{(2)}$	$N^{(007)}$	1.722(5)	$C^{(00D)}$	$C^{(00N)}$	1.387(10)
$P^{(2)}$	$C^{(00D)}$	1.816(6)	$C^{(00F)}$	$C^{(00V)}$	1.388(11)
$P^{(2)}$	$C^{(00F)}$	1.828(7)	$C^{(00F)}$	$C^{(011)}$	1.345(12)
$P^{(1)}$	$N^{(007)}$	1.718(6)	$C^{(00H)}$	$C^{(00T)}$	1.375(10)
$P^{(1)}$	$C^{(008)}$	1.810(6)	$C^{(00I)}$	$C^{(00P)}$	1.388(11)
$P^{(1)}$	$C^{(00E)}$	1.809(6)	$C^{(00J)}$	$C^{(00U)}$	1.358(10)
$P^{(004)}$	$F^{(00G)}$	1.590(8)	$C^{(00K)}$	$C^{(00R)}$	1.375(11)
$P^{(004)}$	$F^{(00G)2}$	1.590(8)	$C^{(00K)}$	$C^{(00S)}$	1.402(11)
$P^{(004)}$	$F^{(00Y)2}$	1.537(7)	$C^{(00L)}$	$C^{(00R)}$	1.389(10)
$P^{(004)}$	$F^{(00Y)}$	1.537(7)	$C^{(00M)}$	$C^{(00S)}$	1.392(9)
$P^{(004)}$	$F^{(012)2}$	1.530(7)	$C^{(00N)}$	$C^{(00X)}$	1.350(12)
$P^{(004)}$	$F^{(012)}$	1.530(7)	$C^{(00O)}$	$C^{(010)}$	1.391(11)
$S^{(005)}$	$C^{(00K)}$	1.770(8)	$C^{(00Q)}$	$C^{(00U)}$	1.400(12)
$S^{(005)}$	$C^{(013)}$	1.802(13)	$C^{(00Q)}$	$C^{(00X)}$	1.355(12)
$N^{(007)}$	$C^{(00C)}$	1.445(8)	$C^{(00T)}$	$C^{(00W)}$	1.366(12)
$C^{(008)}$	$C^{(00H)}$	1.404(9)	$C^{(00V)}$	$C^{(015)}$	1.418(12)
$C^{(008)}$	$C^{(00O)}$	1.379(10)	$C^{(00W)}$	$C^{(010)}$	1.374(12)
$C^{(009)}$	$C^{(00B)}$	1.365(10)	$C^{(011)}$	$C^{(016)}$	1.400(13)
$C^{(009)}$	$C^{(00E)}$	1.411(9)	$C^{(014)}$	$C^{(015)}$	1.329(17)
$C^{(00A)}$	$C^{(00E)}$	1.388(9)	$C^{(014)}$	$C^{(016)}$	1.400(17)
$C^{(00A)}$	$C^{(00P)}$	1.398(10)			

[1]1-X,+Y,3/2-Z; [2]2-X,+Y,1/2-Z

Table 5 Bond Angles for final40s.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$P^{(2)1}$	$Cu^{(01)}$	$P^{(2)}$	139.05(10)	$C^{(00B)}$	$C^{(009)}$	$C^{(00E)}$	122.3(6)
$P^{(2)}$	$Cu^{(01)}$	$P^{(1)}$	73.68(6)	$C^{(00E)}$	$C^{(00A)}$	$C^{(00P)}$	120.4(6)

Table 5 Bond Angles for final40s.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P(2)1	Cu(01)	P(1)1	73.69(6)	C(009)	C(00B)	C(00I)	119.2(7)
P(2)1	Cu(01)	P(1)	130.77(6)	C(00L)	C(00C)	N(007)	120.0(6)
P(2)	Cu(01)	P(1)1	130.77(6)	C(00M)	C(00C)	N(007)	121.0(6)
P(1)	Cu(01)	P(1)1	115.74(9)	C(00M)	C(00C)	C(00L)	119.0(6)
N(007)	P(2)	Cu(01)	90.05(19)	C(00J)	C(00D)	P(2)	121.9(5)
N(007)	P(2)	C(00D)	107.4(3)	C(00J)	C(00D)	C(00N)	118.1(6)
N(007)	P(2)	C(00F)	107.2(3)	C(00N)	C(00D)	P(2)	119.0(5)
C(00D)	P(2)	Cu(01)	119.9(2)	C(009)	C(00E)	P(1)	117.2(5)
C(00D)	P(2)	C(00F)	105.5(3)	C(00A)	C(00E)	P(1)	124.5(5)
C(00F)	P(2)	Cu(01)	123.8(3)	C(00A)	C(00E)	C(009)	117.9(6)
N(007)	P(1)	Cu(01)	89.62(18)	C(00V)	C(00F)	P(2)	122.7(6)
N(007)	P(1)	C(008)	109.0(3)	C(011)	C(00F)	P(2)	118.2(6)
N(007)	P(1)	C(00E)	105.5(3)	C(011)	C(00F)	C(00V)	119.0(8)
C(008)	P(1)	Cu(01)	123.1(2)	C(00T)	C(00H)	C(008)	120.8(7)
C(00E)	P(1)	Cu(01)	119.8(2)	C(00P)	C(00I)	C(00B)	120.0(7)
C(00E)	P(1)	C(008)	106.4(3)	C(00U)	C(00J)	C(00D)	120.9(7)
F(00G)2	P(004)	F(00G)	93.7(7)	C(00R)	C(00K)	S(005)	118.1(6)
F(00Y)	P(004)	F(00G)2	87.6(4)	C(00R)	C(00K)	C(00S)	119.5(7)
F(00Y)2	P(004)	F(00G)	87.6(4)	C(00S)	C(00K)	S(005)	122.3(7)
F(00Y)2	P(004)	F(00G)2	177.4(6)	C(00R)	C(00L)	C(00C)	119.1(7)
F(00Y)	P(004)	F(00G)	177.4(6)	C(00C)	C(00M)	C(00S)	121.7(7)
F(00Y)2	P(004)	F(00Y)	91.2(6)	C(00X)	C(00N)	C(00D)	120.0(7)
F(012)2	P(004)	F(00G)2	86.8(6)	C(008)	C(00O)	C(010)	120.5(7)
F(012)	P(004)	F(00G)	86.7(6)	C(00I)	C(00P)	C(00A)	120.2(7)
F(012)	P(004)	F(00G)2	86.2(5)	C(00X)	C(00Q)	C(00U)	117.9(7)
F(012)2	P(004)	F(00G)	86.2(5)	C(00K)	C(00R)	C(00L)	121.6(7)
F(012)2	P(004)	F(00Y)	96.2(7)	C(00M)	C(00S)	C(00K)	119.1(8)
F(012)2	P(004)	F(00Y)2	91.0(7)	C(00W)	C(00T)	C(00H)	119.7(7)
F(012)	P(004)	F(00Y)	91.0(7)	C(00J)	C(00U)	C(00Q)	120.2(7)
F(012)	P(004)	F(00Y)2	96.2(7)	C(00F)	C(00V)	C(015)	118.7(10)
F(012)	P(004)	F(012)2	169.7(12)	C(010)	C(00W)	C(00T)	120.9(7)
C(00K)	S(005)	C(013)	103.9(4)	C(00N)	C(00X)	C(00Q)	122.8(8)
P(1)	N(007)	P(2)	105.9(3)	C(00W)	C(010)	C(00O)	119.7(8)
C(00C)	N(007)	P(2)	127.9(4)	C(00F)	C(011)	C(016)	123.2(10)
C(00C)	N(007)	P(1)	125.8(4)	C(015)	C(014)	C(016)	121.4(10)
C(00H)	C(008)	P(1)	125.2(5)	C(014)	C(015)	C(00V)	120.9(10)
C(00O)	C(008)	P(1)	116.4(5)	C(011)	C(016)	C(014)	116.7(11)
C(00O)	C(008)	C(00H)	118.4(6)				

[1]1-X,+Y,3/2-Z; [2]2-X,+Y,1/2-Z

Table 6 Torsion Angles for final40s.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu(01)	P(2)	N(007)	P(1)	7.7(3)	C(00B)	C(009)	C(00E)	C(00A)	0.4(10)
Cu(01)	P(2)	N(007)	C(00C)	-179.4(5)	C(00B)	C(00I)	C(00P)	C(00A)	1.9(11)
Cu(01)	P(2)	C(00D)	C(00J)	73.4(6)	C(00C)	C(00L)	C(00R)	C(00K)	1.5(10)
Cu(01)	P(2)	C(00D)	C(00N)	-95.0(6)	C(00C)	C(00M)	C(00S)	C(00K)	-1.6(11)
Cu(01)	P(2)	C(00F)	C(00V)	169.1(6)	C(00D)	P(2)	N(007)	P(1)	129.2(3)
Cu(01)	P(2)	C(00F)	C(011)	-13.8(8)	C(00D)	P(2)	N(007)	C(00C)	-58.0(6)
Cu(01)	P(1)	N(007)	P(2)	-7.6(3)	C(00D)	P(2)	C(00F)	C(00V)	25.3(8)
Cu(01)	P(1)	N(007)	C(00C)	179.3(5)	C(00D)	P(2)	C(00F)	C(011)	-157.6(7)
Cu(01)	P(1)	C(008)	C(00H)	161.7(5)	C(00D)	C(00J)	C(00U)	C(00Q)	-1.0(11)
Cu(01)	P(1)	C(008)	C(00O)	-18.9(7)	C(00D)	C(00N)	C(00X)	C(00Q)	0.4(16)
Cu(01)	P(1)	C(00E)	C(009)	-37.2(6)	C(00E)	P(1)	N(007)	P(2)	-128.6(3)
Cu(01)	P(1)	C(00E)	C(00A)	135.4(5)	C(00E)	P(1)	N(007)	C(00C)	58.4(6)
P(2)	N(007)	C(00C)	C(00L)	-64.3(8)	C(00E)	P(1)	C(008)	C(00H)	-54.1(6)
P(2)	N(007)	C(00C)	C(00M)	117.8(7)	C(00E)	P(1)	C(008)	C(00O)	125.4(6)
P(2)	C(00D)	C(00J)	C(00U)	-169.2(6)	C(00E)	C(009)	C(00B)	C(00I)	0.0(11)
P(2)	C(00D)	C(00N)	C(00X)	169.9(8)	C(00E)	C(00A)	C(00P)	C(00I)	-1.5(11)
P(2)	C(00F)	C(00V)	C(015)	176.9(8)	C(00F)	P(2)	N(007)	P(1)	-117.9(3)

Table 6 Torsion Angles for final40s.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P(2)	C(00F)	C(011)	C(016)	-175.5(10)	C(00F)	P(2)	N(007)	C(00C)	54.9(6)
P(1)	N(007)	C(00C)	C(00L)	107.2(7)	C(00F)	P(2)	C(00D)	C(00J)	-141.1(6)
P(1)	N(007)	C(00C)	C(00M)	-70.7(8)	C(00F)	P(2)	C(00D)	C(00N)	50.5(7)
P(1)	C(008)	C(00H)	C(00T)	178.5(6)	C(00F)	C(00V)	C(015)	C(014)	0.4(19)
P(1)	C(008)	C(00O)	C(010)	-177.6(7)	C(00F)	C(011)	C(016)	C(014)	-3.4(19)
S(005)	C(00K)	C(00R)	C(00L)	-177.8(5)	C(00H)	C(008)	C(00O)	C(010)	1.9(12)
S(005)	C(00K)	C(00S)	C(00M)	177.6(5)	C(00H)	C(00T)	C(00W)	C(010)	3.5(14)
N(007)	P(2)	C(00D)	C(00J)	-27.0(6)	C(00J)	C(00D)	C(00N)	C(00X)	1.1(13)
N(007)	P(2)	C(00D)	C(00N)	164.6(6)	C(00L)	C(00C)	C(00M)	C(00S)	0.9(10)
N(007)	P(2)	C(00F)	C(00V)	-88.9(8)	C(00M)	C(00C)	C(00L)	C(00R)	-0.8(10)
N(007)	P(2)	C(00F)	C(011)	88.2(7)	C(00N)	C(00D)	C(00J)	C(00U)	-0.8(11)
N(007)	P(1)	C(008)	C(00H)	59.2(7)	C(00O)	C(008)	C(00H)	C(00T)	-0.9(11)
N(007)	P(1)	C(008)	C(00O)	-121.3(6)	C(00P)	C(00A)	C(00E)	P(1)	-172.2(5)
N(007)	P(1)	C(00E)	C(009)	61.4(5)	C(00P)	C(00A)	C(00E)	C(009)	0.4(9)
N(007)	P(1)	C(00E)	C(00A)	-125.9(5)	C(00R)	C(00K)	C(00S)	C(00M)	2.2(10)
N(007)	C(00C)	C(00L)	C(00R)	-178.8(6)	C(00S)	C(00K)	C(00R)	C(00L)	-2.2(11)
N(007)	C(00C)	C(00M)	C(00S)	178.8(6)	C(00T)	C(00W)	C(010)	C(00O)	-2.6(15)
C(008)	P(1)	N(007)	P(2)	117.5(3)	C(00U)	C(00Q)	C(00X)	C(00N)	-2.1(15)
C(008)	P(1)	N(007)	C(00C)	-55.6(6)	C(00V)	C(00F)	C(011)	C(016)	1.8(16)
C(008)	P(1)	C(00E)	C(009)	177.1(5)	C(00X)	C(00Q)	C(00U)	C(00J)	2.5(13)
C(008)	P(1)	C(00E)	C(00A)	-10.3(6)	C(011)	C(00F)	C(00V)	C(015)	-0.2(15)
C(008)	C(00H)	C(00T)	C(00W)	-1.8(12)	C(013)	S(005)	C(00K)	C(00R)	-156.0(6)
C(008)	C(00O)	C(010)	C(00W)	-0.2(15)	C(013)	S(005)	C(00K)	C(00S)	28.6(7)
C(009)	C(00B)	C(00I)	C(00P)	-1.2(11)	C(015)	C(014)	C(016)	C(011)	4(2)
C(00B)	C(009)	C(00E)	P(1)	173.5(6)	C(016)	C(014)	C(015)	C(00V)	-2(2)

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for final40s.

Atom	*x*	*y*	*z*	U(eq)
H(009)	6586.91	5473.34	7491.61	33
H(00A)	4050.5	4763.78	5801.58	30
H(00B)	7004.47	3855.13	7727.31	39
H(00H)	4595.02	6114.41	5082.59	39
H(00I)	5950.45	2659.05	6989.64	45
H(00J)	8123.89	6492.24	7426.34	33
H(00L)	6295.7	8257.13	5474.66	36
H(00M)	7347.9	5639.33	6332.67	34
H(00N)	8058.82	9295.43	7997.94	53
H(00O)	2792.42	7429.58	6193.62	48
H(00P)	4443.36	3115.38	6050.3	41
H(00Q)	10764.36	7631.87	8890.51	52
H(00R)	7231.31	7944.65	4659.83	39
H(00S)	8283.14	5331.74	5515.59	42
H(00T)	3092.4	6361.29	4104.93	44
H(00U)	9867.99	6295.36	8225.39	45
H(00V)	8039.34	9322.27	6686.27	68
H(00W)	1406.43	7037.57	4180.35	55
H(00X)	9796.22	9083.71	8778.38	65
H(010)	1267.75	7629.58	5207.34	65
H(011)	4712.49	9373.27	6542.87	68
H(01A)	8829.53	4992.12	3879.92	106
H(01B)	7844.92	4866.2	4240.08	106
H(01C)	9155.24	4881.15	4687.18	106
H(014)	6078.68	11523.81	5698.95	104
H(015)	7802.89	10787.94	6054.79	97
H(016)	4444.49	10788.76	5875.11	104

Table 8 Solvent masks information for final40s.

Number	X	Y	Z	Volume	Electron count	Content

Table 8 Solvent masks information for final40s.

Number	X	Y	Z	Volume	Electron count	Content
1	0.473	0.000	-0.556	712.5	306.3	?

5.2 Details and Tables for 2

Single crystals of C64H59AgF6N2O0.5P5S2 [first_25] were submitted for single crystal X-ray determination. A suitable crystal was selected and mounted on a MiTeGen tip using Parabol oil and placed on a Bruker APEX-II Photon 100 diffractometer. The crystal was kept at 150.0 K during data collection. Using Olex2[4], the structure was solved with the XT[5] structure solution program using Intrinsic Phasing and refined with the XL[6] refinement package using Least Squares minimisation. Due to severe solvent disorder, the SQUEEZE algorithm was utilised, resulting in ca. 75 electrons being removed for solvent accessible void space. This accounts for two ether molecules per asymmetric unit. Furthermore, due to the end of life of the Photon 100 detector, there were unaccounted for overloads at low angle that could not be used in the data refinement stage. These have given rise to the B Alerts in the checkcif report.

Crystal Data for C63.985H58.9525AgF6N2O0.5P5S2 (M =1304.74 g/mol): triclinic, space group P-1 (no. 2), a = 13.5820(14) Å, b = 21.259(3) Å, c = 23.026(3) Å, α = 87.876(6)°, β = 78.360(5)°, γ = 82.975(4)°, V = 6462.2(14) Å3, Z = 4, T = 150.0 K, μ(MoKα) = 0.558 mm-1, Dcalc = 1.341 g/cm3, 111867 reflections measured (0.504° ≤ 2Θ ≤ 52.872°), 26074 unique (Rint = 0.0620, Rsigma = 0.0546) which were used in all calculations. The final R1 was 0.0440 (I > 2σ(I)) and wR2 was 0.1179 (all data).

Table 1 Crystal data and structure refinement for first_25.

Identification code	first_25
Empirical formula	$C_{63.98}H_{58.95}AgF_6N_2O_{0.5}P_5S_2$
Formula weight	1304.74
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	13.5820(14)
b/Å	21.259(3)
c/Å	23.026(3)
α/°	87.876(6)
β/°	78.360(5)
γ/°	82.975(4)
Volume/Å^3	6462.2(14)
Z	4
ρ_{calc}g/cm^3	1.341
μ/mm^{-1}	0.558
F(000)	2675.0
Crystal size/mm^3	0.2 × 0.05 × 0.05
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	0.504 to 52.872
Index ranges	-16 ≤ h ≤ 16, -26 ≤ k ≤ 26, -28 ≤ l ≤ 28
Reflections collected	111867
Independent reflections	26074 [R_{int} = 0.0620, R_{sigma} = 0.0546]
Data/restraints/parameters	26074/1/1493
Goodness-of-fit on F^2	0.984
Final R indexes [I>=2σ (I)]	R_1 = 0.0440, wR_2 = 0.1029
Final R indexes [all data]	R_1 = 0.0755, wR_2 = 0.1179
Largest diff. peak/hole / e Å^{-3}	0.59/-0.68

Table 2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for first_25. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Ag(01)	1183.1(2)	2160.7(2)	6373.6(2)	25.29(7)
Ag(02)	5237.8(2)	2894.7(2)	2022.9(2)	23.44(7)
P(003)	5912.2(6)	3817.3(4)	2386.3(3)	18.73(17)
P(004)	4586.8(6)	3911.7(3)	1580.5(3)	19.15(17)
P(005)	620.3(6)	3137.3(4)	5819.1(4)	21.38(17)
P(006)	2065.5(6)	1119.5(4)	5992.0(4)	20.94(17)
P(007)	616.2(6)	1241.4(4)	7058.1(4)	22.27(18)
P(008)	4382.0(6)	2015.7(3)	2529.3(3)	20.10(17)
P(009)	1944.3(6)	3117.7(4)	6618.8(3)	19.17(17)
S(00A)	4602.9(8)	-1289.6(4)	1993.4(4)	39.0(2)
P(00B)	5940.1(6)	1846.1(4)	1510.5(4)	21.35(18)
S(00C)	5333.0(8)	7130.8(4)	1640.3(4)	35.9(2)
P(00D)	-2158.2(7)	1972.4(4)	5432.2(4)	34.3(2)
S(00E)	1567.2(7)	6392.7(4)	5880.9(5)	39.1(2)
S(00F)	1600.8(11)	-2133.8(5)	6681.7(6)	33.3(5)
P(00G)	1464.9(9)	3117.6(6)	10312.4(5)	52.3(3)
F(00I)	-3135.7(17)	2012.4(12)	5135.3(11)	53.6(6)
N(00J)	5140(2)	1465.7(11)	2057.8(11)	21.0(6)
F(00K)	-2289.0(17)	2726.0(10)	5472.4(10)	45.6(5)
C(00L)	-624(2)	3582.4(15)	5976.5(15)	26.0(7)
N(00M)	5339.1(19)	4315.8(11)	1916.8(11)	19.0(5)
C(00N)	1440(2)	4248.3(13)	6044.9(13)	19.5(6)
C(00O)	5593(3)	1730.4(15)	800.5(14)	26.3(7)
C(00P)	5428(2)	4120.8(15)	3131.5(14)	24.1(7)
F(00Q)	-2013(2)	1219.5(11)	5400.1(14)	73.2(9)
C(00R)	6287(3)	5892.4(14)	1547.6(14)	24.7(7)
C(00S)	1757(2)	848.5(14)	5320.3(14)	23.5(7)
C(00T)	3077(2)	1929.8(15)	2509.2(14)	24.7(7)
F(00U)	2240(2)	3501.3(15)	9863.2(13)	87.3(10)
C(00V)	4771(3)	-484.8(15)	2051.6(15)	28.8(8)
C(00W)	4922(3)	4059.3(14)	792.9(14)	24.3(7)
C(00X)	5506(3)	4733.4(15)	3305.9(15)	27.9(7)
C(00Y)	6263(3)	5238.5(14)	1608.6(14)	25.1(7)
C(00Z)	994(2)	3169.4(15)	5015.8(14)	23.8(7)
C(010)	4746(3)	2082(2)	668.4(17)	49.3(11)
C(011)	906(3)	2687(2)	4102.7(17)	45.8(10)
F(012)	-2873.6(18)	1927.8(12)	6072.4(10)	56.9(7)
F(013)	710.3(19)	2736.0(13)	10771.0(12)	68.8(8)
C(014)	1500(2)	3469.6(14)	7343.6(14)	23.7(7)
F(015)	-1183.3(17)	1952.6(12)	5730.2(10)	52.5(6)
C(016)	3786(3)	3054.7(15)	5836.4(14)	26.6(7)
N(017)	1422(2)	720.5(11)	6579.8(11)	21.8(6)
N(018)	1391.1(19)	3574.0(11)	6113.7(11)	20.5(6)
C(019)	3284(2)	3210.6(13)	6416.2(13)	18.8(6)
C(01A)	4898(3)	3362.6(18)	6642.0(16)	36.5(9)
C(01B)	-527(2)	853.5(14)	7242.8(14)	24.4(7)
C(01C)	5423(3)	6300.3(14)	1740.7(14)	23.3(7)
C(01D)	816(3)	1515.5(17)	8777.5(16)	40.3(9)
C(01E)	3297(2)	4294.4(15)	1807.0(14)	24.2(7)
C(01F)	8797(3)	3715.5(17)	1480.6(16)	35.6(9)
C(01G)	7249(2)	3920.0(14)	2207.9(14)	21.9(7)
C(01H)	666(3)	5331.2(15)	6172.6(15)	28.0(7)
C(01I)	4552(2)	1825.8(13)	3280.5(13)	20.6(7)
C(01J)	5385(3)	3210.2(16)	6066.3(17)	34.4(8)
C(01K)	-1227(3)	987.3(17)	6876.2(15)	32.4(8)
C(01L)	1844(3)	1393.7(19)	8762.5(17)	44.3(10)

Table 2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for first_25. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C(01M)	7802(3)	4092.7(15)	2610.2(15)	27.6(7)
C(01N)	3858(3)	3359.0(15)	6817.4(14)	27.3(7)
C(01O)	4616(3)	561.7(15)	1610.9(15)	29.0(8)
C(01P)	2426(2)	5128.5(15)	5740.7(14)	25.7(7)
C(01Q)	5372(2)	4994.9(13)	1874.1(13)	18.8(6)
C(01R)	598(2)	4687.2(15)	6243.3(15)	25.9(7)
C(01S)	441(3)	1431.5(16)	8268.0(15)	34.2(8)
C(01T)	4517(2)	5406.3(14)	2098.1(14)	23.4(7)
F(01U)	2340(2)	2908.2(16)	10679.0(16)	91.5(10)
F(01V)	602(3)	3358.0(18)	9977.6(18)	114.1(14)
C(01W)	4950(3)	1792.1(17)	4423.4(16)	37.0(9)
C(01X)	4993(2)	808.3(14)	2060.6(13)	21.9(7)
C(01Y)	3404(2)	859.9(15)	5941.3(13)	23.4(7)
C(01Z)	-1934(3)	4370(2)	5761.7(19)	48.1(11)
O(020)	-1755(2)	-344.7(14)	9341.3(13)	54.5(8)
C(021)	2587(3)	2384.2(18)	2179.3(16)	36.1(9)
C(022)	4541(3)	6056.5(14)	2025.3(14)	25.2(7)
C(023)	-1007(3)	4008.9(18)	5582.1(16)	36.6(9)
C(024)	5058(3)	1189.5(18)	5900.8(16)	36.0(9)
C(025)	7764(3)	3726.1(15)	1640.2(15)	29.1(8)
C(026)	1488(2)	34.2(14)	6644.7(15)	25.1(7)
C(027)	4820(3)	3057.9(15)	5663.7(16)	30.4(8)
F(028)	1161(2)	3731.5(14)	10711.3(14)	87.6(10)
C(029)	5540(3)	1691.6(15)	3376.8(14)	26.9(7)
C(02A)	5079(3)	4931.1(18)	3877.7(16)	37.5(9)
C(02B)	1234(3)	4294.8(18)	8063.7(16)	39.2(9)
C(02C)	658(3)	2709.7(18)	4716.5(16)	36.9(9)
C(02D)	8846(3)	4074.0(17)	2448.2(17)	36.3(9)
C(02E)	2542(3)	1459.8(17)	2813.7(16)	34.7(8)
C(02F)	1355(3)	4896(2)	2250.5(19)	48.5(10)
C(02G)	2353(2)	4480.4(14)	5791.6(14)	23.4(7)
C(02H)	4784(4)	-1623.8(17)	2699.2(17)	56.6(13)
C(02I)	2786(3)	4148.8(18)	2366.9(16)	39.3(9)
C(02J)	740(3)	904.4(17)	5286.6(16)	33.4(8)
C(02K)	9346(3)	3889.0(17)	1885.5(17)	36.7(9)
C(02L)	1204(5)	-325(3)	6192(3)	33.2(14)
C(02M)	2476(3)	651.8(17)	4823.7(15)	33.8(8)
C(02N)	3844(3)	231.7(16)	5870.4(15)	29.9(8)
C(02O)	5239(3)	403.0(14)	2511.9(14)	27.3(7)
C(02P)	1505(3)	3109.9(19)	3783.6(16)	41.2(10)
C(02Q)	1610(3)	4083.4(15)	7490.8(14)	27.8(7)
C(02R)	4021(3)	1332.3(16)	5966.8(14)	28.2(8)
C(02S)	-1606(4)	-1(2)	9825(2)	65.3(14)
C(02T)	5496(4)	4108(2)	-432.9(17)	55.8(12)
C(02U)	6158(4)	1322(2)	374.1(19)	65.9(15)
C(02V)	1582(3)	5566.1(15)	5926.9(15)	26.0(7)
C(02W)	1817(3)	4456(2)	2589.2(19)	52.7(11)
C(02X)	3767(3)	1946.2(16)	3767.3(15)	29.8(8)
C(02Y)	-2059(3)	661.8(19)	6945.2(19)	43.5(10)
C(02Z)	1167(3)	540.6(18)	4286.8(17)	40.3(9)
C(030)	4511(3)	-74.4(16)	1604.2(15)	33.4(8)
C(031)	1867(3)	5039(2)	1689(2)	57.8(12)
F(032)	1807(3)	2502.8(15)	9925.5(15)	100.1(12)
C(033)	7202(3)	1413.0(15)	1418.0(14)	25.2(7)
C(034)	757(4)	3896(2)	8485.8(18)	52.8(12)
C(036)	1586(3)	2367(2)	2152(2)	55.4(12)
C(037)	2870(3)	6494.8(17)	5606.3(18)	41.2(9)
C(038)	4572(3)	4522(2)	4278.0(17)	45.0(10)
C(039)	4583(4)	3898(2)	-172.0(17)	54.6(12)
C(03A)	7428(3)	753.0(16)	1431.8(16)	35.0(8)

Table 2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for first_25. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C(03B)	5122(3)	-237.9(15)	2507.5(15)	30.5(8)
C(03C)	8422(3)	478.7(17)	1331.0(17)	38.7(9)
C(03D)	2828(3)	4742(2)	1468.5(18)	45.6(10)
C(03E)	437(3)	750.4(19)	4778.8(17)	42.1(9)
C(03F)	5731(3)	1672.6(17)	3945.1(16)	35.9(9)
C(03G)	5841(3)	4260.1(16)	529.9(15)	32.0(8)
C(03H)	1096(3)	1230.2(15)	7745.8(14)	25.7(7)
C(03I)	6124(3)	4285.3(19)	-81.4(16)	44.7(10)
C(03L)	1532(3)	1452(2)	2787.3(19)	52.4(11)
C(03M)	8004(3)	1777.1(17)	1298.2(17)	35.0(8)
C(03N)	4293(3)	3869.6(18)	438.7(16)	40.1(9)
C(03O)	8994(3)	1499.5(19)	1186.7(19)	44.8(10)
C(03P)	5481(3)	573.3(19)	5826.4(16)	37.8(9)
C(03Q)	-2104(3)	3888(2)	6718(2)	60.5(13)
C(03R)	9206(3)	849.2(19)	1205.7(17)	40.4(9)
C(03S)	1780(5)	-309(3)	7096(3)	31.4(14)
C(03T)	2131(3)	1121.0(18)	7738.6(16)	35.8(8)
C(03V)	4462(4)	2036(2)	133.5(18)	62.3(14)
C(03W)	-2479(3)	4313(2)	6327(2)	54.9(12)
C(03Z)	-1196(3)	3517(2)	6542.7(18)	45.7(10)
C(040)	-2213(3)	210(2)	7385(2)	49.3(11)
C(041)	1568(4)	-1303(2)	6695(3)	24.0(11)
C(042)	5044(4)	1648(3)	-291.4(19)	66.6(15)
C(043)	2492(3)	1197(2)	8251.8(18)	46.2(10)
C(044)	1849(3)	3560(2)	4076.6(17)	49.5(11)
C(046)	-690(3)	397.6(17)	7685.7(16)	35.8(9)
C(047)	1813(5)	-967(3)	7136(2)	31.3(12)
C(049)	2173(3)	503.3(19)	4307.6(16)	41.9(10)
C(04B)	4879(3)	89.3(18)	5815.1(17)	38.7(9)
C(04C)	6622(3)	7286.1(18)	1404(2)	53.6(12)
C(04D)	-1545(3)	82.4(19)	7767(2)	49.7(11)
C(04E)	1063(3)	1901(3)	2459(2)	60.9(13)
C(04F)	3969(3)	1927.7(18)	4335.5(15)	38.5(9)
C(04H)	1257(5)	-971(2)	6228(3)	35.7(13)
C(8)	1013(3)	3080.5(18)	7775.9(16)	43.1(10)
C(10)	5879(4)	1283(3)	-172(2)	89(2)
F(1)	-1444.4(17)	2021.3(11)	4791.8(9)	46.5(6)
C(4)	4914(3)	3714.1(18)	3540.7(15)	33.8(8)
C(9)	4485(3)	3916(2)	4112.7(17)	46.5(10)
C(1)	1591(3)	3596.1(19)	4691.6(16)	44.5(10)
C(0AA)	641(4)	3295(2)	8346.0(19)	64.8(14)
C(1AA)	-1209(4)	612(2)	9597(2)	75.1(16)
C(3)	-2095(5)	-940(2)	9511(2)	72.7(15)
C(3AA)	-2139(5)	-1289(3)	8982(2)	77.3(16)
S(4AA)	1792(3)	-2028.2(19)	7171.8(18)	35.8(15)
C(2)	1826(5)	-2384(3)	7402(3)	41.5(19)
C(2BA)	1158(14)	-969(9)	6517(8)	31(4)
C(1BA)	1630(13)	-1210(9)	6945(8)	18(4)
C(0BA)	2124(12)	-835(7)	7256(7)	21(4)
C(5)	2043(11)	-175(7)	7133(7)	12(4)
C(3BA)	1057(16)	-296(10)	6417(8)	29(5)
C(4AA)	1343(17)	-2385(12)	6601(9)	71(8)

Table 3 Anisotropic Displacement Parameters (Å²×10³) for first_25. 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}
Ag(01)	31.62(15)	14.70(12)	29.68(14)	0.30(9)	-5.97(11)	-3.66(10)
Ag(02)	31.62(15)	12.92(11)	26.61(13)	2.93(9)	-6.9(1)	-4.99(10)
P(003)	21.4(4)	15.8(4)	20.1(4)	1.8(3)	-6.9(3)	-2.8(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for first_25. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P(004)	24.3(5)	14.5(4)	20.5(4)	3.3(3)	-7.4(3)	-5.8(3)
P(005)	21.6(4)	19.5(4)	24.6(4)	0.3(3)	-7.3(3)	-3.9(3)
P(006)	22.5(4)	15.8(4)	23.4(4)	-0.2(3)	-1.5(3)	-3.0(3)
P(007)	23.6(5)	18.3(4)	23.9(4)	1.3(3)	-2.4(3)	-2.8(3)
P(008)	25.0(5)	13.6(4)	20.8(4)	1.1(3)	-2.4(3)	-2.3(3)
P(009)	20.7(4)	15.4(4)	21.9(4)	0.1(3)	-6.2(3)	-1.4(3)
S(00A)	60.7(7)	17.1(4)	38.6(5)	-3.6(4)	-3.1(5)	-12.9(4)
P(00B)	25.2(5)	15.6(4)	21.8(4)	1.1(3)	-2.1(3)	-1.5(3)
S(00C)	49.9(6)	12.9(4)	43.7(5)	0.1(3)	-5.3(4)	-5.7(4)
P(00D)	25.2(5)	30.2(5)	44.5(6)	7.8(4)	-2.1(4)	-1.7(4)
S(00E)	33.3(5)	18.9(4)	65.0(7)	11.1(4)	-12.0(5)	-2.5(4)
S(00F)	44.4(9)	14.0(6)	41.0(9)	-1.9(5)	-7.1(6)	-3.1(5)
P(00G)	38.3(7)	59.3(7)	51.8(7)	4.9(6)	6.6(5)	-3.3(6)
F(00I)	36.8(14)	66.8(16)	63.3(16)	9.5(12)	-17.3(12)	-20.5(12)
N(00J)	25.0(15)	14.5(12)	21.4(13)	-0.3(10)	-1.0(11)	-0.2(11)
F(00K)	43.7(14)	33.0(12)	57.8(14)	0.8(10)	-7.8(11)	-0.1(10)
C(00L)	23.8(18)	24.2(16)	33.0(18)	-0.7(14)	-10.1(15)	-6.4(14)
N(00M)	21.5(14)	13.9(12)	23.2(13)	1.9(10)	-7.7(11)	-3.8(11)
C(00N)	21.9(17)	15.9(14)	22.0(16)	1.8(12)	-8.6(13)	-1.0(13)
C(00O)	31(2)	24.3(16)	21.4(16)	2.6(13)	-1.7(14)	-2.4(15)
C(00P)	20.2(17)	29.7(17)	23.0(16)	-1.2(13)	-7.4(13)	0.1(14)
F(00Q)	66.9(19)	27.6(12)	113(2)	5.3(13)	8.7(16)	-5.9(12)
C(00R)	25.1(18)	19.7(15)	31.2(18)	1.6(13)	-6.5(14)	-8.7(14)
C(00S)	25.7(18)	16.4(15)	25.9(17)	-0.4(12)	-0.7(14)	0.4(13)
C(00T)	26.3(19)	24.4(16)	23.0(16)	-4.5(13)	-3.8(14)	-2.3(14)
F(00U)	88(2)	90(2)	72(2)	-3.3(16)	30.6(17)	-39.4(18)
C(00V)	36(2)	17.3(15)	30.9(18)	-2.8(13)	-0.7(15)	-5.3(14)
C(00W)	34(2)	17.2(15)	23.7(16)	1.9(12)	-10.7(14)	-2.5(14)
C(00X)	29(2)	27.2(17)	28.9(18)	-0.8(14)	-12.0(15)	2.9(15)
C(00Y)	24.6(18)	18.7(15)	33.1(18)	1.0(13)	-7.7(14)	-3.7(14)
C(00Z)	19.2(17)	28.6(17)	23.6(16)	-3.5(13)	-7.2(13)	3.4(14)
C(010)	62(3)	50(2)	32(2)	-9.5(18)	-16(2)	22(2)
C(011)	51(3)	54(3)	35(2)	-22.4(19)	-10.4(19)	-4(2)
F(012)	41.5(14)	69.0(17)	50.2(14)	19.8(12)	6.8(11)	-0.4(12)
F(013)	43.9(16)	72.3(18)	77.6(19)	21.8(15)	10.5(13)	-2.0(13)
C(014)	22.6(18)	23.2(16)	25.6(17)	-0.6(13)	-7.2(14)	-0.4(14)
F(015)	31.8(13)	65.6(16)	58.7(15)	18.8(12)	-13.1(11)	0.1(11)
C(016)	30(2)	24.3(16)	26.5(17)	-3.8(13)	-8.0(15)	-4.1(14)
N(017)	24.5(15)	15.2(12)	24.2(14)	1.9(10)	-2.6(11)	-1.2(11)
N(018)	20.5(14)	16.5(12)	26.6(14)	2.6(10)	-10.1(11)	-2.7(11)
C(019)	17.9(16)	15.5(14)	22.9(16)	1.2(12)	-6.2(13)	1.7(12)
C(01A)	28(2)	47(2)	38(2)	-1.4(17)	-13.1(17)	-8.3(17)
C(01B)	22.9(18)	21.2(16)	26.9(17)	0.6(13)	0.2(14)	-2.8(14)
C(01C)	33(2)	14.8(15)	24.3(16)	-0.6(12)	-9.9(14)	-4.0(14)
C(01D)	57(3)	38(2)	24.7(19)	-2.7(15)	-1.2(18)	-8.4(19)
C(01E)	20.8(17)	24.8(16)	29.1(17)	2.6(13)	-7.7(14)	-7.1(14)
C(01F)	30(2)	34.5(19)	36(2)	-5.8(16)	3.7(16)	4.5(16)
C(01G)	22.2(17)	15.8(14)	26.9(17)	-0.6(12)	-4.9(14)	1.0(13)
C(01H)	21.0(18)	21.3(16)	41(2)	-2.5(14)	-7.3(15)	5.0(14)
C(01I)	28.9(19)	11.9(14)	20.6(15)	-0.9(11)	-1.9(13)	-6.0(13)
C(01J)	20.4(19)	29.5(18)	50(2)	-0.4(16)	-1.8(17)	1.9(15)
C(01K)	28(2)	35.4(19)	32.7(19)	1.2(15)	-4.5(16)	-0.6(16)
C(01L)	61(3)	47(2)	32(2)	5.0(17)	-17(2)	-21(2)
C(01M)	25.9(19)	28.8(17)	27.8(18)	-6.0(14)	-5.9(15)	0.7(15)
C(01N)	28.3(19)	30.9(18)	24.0(17)	-0.4(14)	-8.0(14)	-4.1(15)
C(01O)	38(2)	21.8(16)	29.4(18)	1.4(14)	-10.1(16)	-5.8(15)
C(01P)	20.9(18)	24.9(17)	31.0(18)	7.9(14)	-3.9(14)	-5.9(14)
C(01Q)	24.4(17)	11.4(13)	22.1(15)	1.3(11)	-7.4(13)	-3.3(12)
C(01R)	18.9(18)	24.3(17)	34.8(19)	-1.9(14)	-5.2(14)	-3.2(14)
C(01S)	40(2)	31.7(19)	29.2(19)	-1.0(15)	-3.6(16)	-1.2(16)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for first_25. 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}
$C^{(01T)}$	26.0(18)	19.3(15)	24.5(17)	-1.3(12)	-2.7(14)	-4.7(14)
$F^{(01U)}$	53.4(19)	94(2)	130(3)	18(2)	-31.3(19)	-5.3(17)
$F^{(01V)}$	106(3)	122(3)	134(3)	68(3)	-69(2)	-38(2)
$C^{(01W)}$	50(3)	41(2)	24.5(18)	3.4(15)	-13.3(17)	-15.8(19)
$C^{(01X)}$	24.4(18)	16.0(15)	23.7(16)	0.1(12)	-1.2(13)	-2.6(13)
$C^{(01Y)}$	21.3(18)	26.1(16)	21.8(16)	-1.1(13)	-1.9(13)	-2.6(14)
$C^{(01Z)}$	39(3)	57(3)	48(3)	-6(2)	-21(2)	18(2)
$O^{(020)}$	60(2)	48.9(17)	51.9(18)	1.1(14)	-1.4(15)	-10.8(15)
$C^{(021)}$	30(2)	42(2)	36(2)	5.0(16)	-9.5(16)	-0.2(17)
$C^{(022)}$	28.4(19)	20.0(16)	25.6(17)	-4.6(13)	-3.5(14)	2.1(14)
$C^{(023)}$	30(2)	47(2)	34(2)	-2.7(16)	-13.9(16)	5.5(17)
$C^{(024)}$	28(2)	46(2)	36(2)	12.1(17)	-6.7(16)	-14.5(18)
$C^{(025)}$	30(2)	27.5(17)	30.8(18)	-6.6(14)	-8.3(15)	-0.6(15)
$C^{(026)}$	21.9(18)	16.6(15)	34.2(18)	4.8(13)	-0.6(14)	-1.3(13)
$C^{(027)}$	30(2)	22.3(17)	35.5(19)	-5.3(14)	0.8(16)	0.5(15)
$F^{(028)}$	87(2)	69.4(19)	89(2)	-10.6(16)	24.1(18)	-6.2(17)
$C^{(029)}$	26.7(19)	27.7(17)	26.4(17)	-1.1(14)	-4.5(14)	-4.4(15)
$C^{(02A)}$	40(2)	41(2)	31(2)	-14.1(16)	-14.2(17)	14.6(18)
$C^{(02B)}$	46(2)	32(2)	38(2)	-13.4(16)	-12.1(18)	8.7(18)
$C^{(02C)}$	36(2)	44(2)	33(2)	-10.2(16)	-5.5(16)	-8.4(18)
$C^{(02D)}$	26(2)	41(2)	45(2)	-7.8(17)	-13.2(17)	-3.0(17)
$C^{(02E)}$	36(2)	36(2)	34(2)	3.0(16)	-4.7(16)	-15.1(17)
$C^{(02F)}$	28(2)	59(3)	55(3)	-3(2)	-6(2)	4(2)
$C^{(02G)}$	19.4(17)	22.2(16)	27.8(17)	4.3(13)	-4.6(14)	-1.2(13)
$C^{(02H)}$	109(4)	19.5(18)	38(2)	0.6(16)	-2(2)	-17(2)
$C^{(02I)}$	36(2)	43(2)	33(2)	13.1(17)	1.4(17)	-0.4(18)
$C^{(02J)}$	27(2)	39(2)	32.8(19)	-11.7(16)	-7.1(16)	7.8(16)
$C^{(02K)}$	18.5(19)	36(2)	54(2)	-2.5(17)	-5.4(17)	-1.9(16)
$C^{(02L)}$	55(4)	21(3)	29(4)	-1(3)	-20(3)	-8(2)
$C^{(02M)}$	27(2)	39(2)	33(2)	-1.6(16)	-5.4(16)	1.4(16)
$C^{(02N)}$	25.8(19)	28.9(18)	32.7(19)	-4.1(14)	-0.8(15)	-1.5(15)
$C^{(02O)}$	38(2)	15.5(15)	28.6(18)	-1.3(13)	-7.2(15)	-3.2(14)
$C^{(02P)}$	40(2)	53(2)	26.6(19)	-3.9(17)	-6.5(17)	11.6(19)
$C^{(02Q)}$	30(2)	26.9(17)	27.3(18)	-1.7(14)	-8.1(15)	-0.5(15)
$C^{(02R)}$	33(2)	26.5(17)	25.5(17)	3.8(14)	-6.9(15)	-6.2(15)
$C^{(02S)}$	78(4)	55(3)	55(3)	-9(2)	6(3)	-7(3)
$C^{(02T)}$	87(4)	62(3)	21(2)	1.9(19)	-12(2)	-21(3)
$C^{(02U)}$	57(3)	94(4)	43(3)	-33(2)	-24(2)	36(3)
$C^{(02V)}$	26.7(19)	19.7(16)	33.2(18)	6.0(13)	-10.1(15)	-3.9(14)
$C^{(02W)}$	36(2)	72(3)	41(2)	10(2)	8.1(19)	1(2)
$C^{(02X)}$	28(2)	30.3(18)	30.1(18)	-0.1(14)	-3.2(15)	-4.1(15)
$C^{(02Y)}$	28(2)	47(2)	57(3)	-8(2)	-9.4(19)	-4.4(18)
$C^{(02Z)}$	45(3)	43(2)	34(2)	-10.0(17)	-15.2(18)	5.2(19)
$C^{(030)}$	46(2)	28.1(18)	30.9(19)	-4.2(15)	-11.4(17)	-13.9(17)
$C^{(031)}$	43(3)	68(3)	58(3)	14(2)	-16(2)	18(2)
$F^{(032)}$	119(3)	79(2)	85(2)	-27.7(18)	36(2)	-31(2)
$C^{(033)}$	25.7(19)	23.2(16)	24.4(17)	-1.3(13)	-2.4(14)	2.4(14)
$C^{(034)}$	67(3)	55(3)	28(2)	-10.0(19)	8(2)	1(2)
$C^{(036)}$	34(3)	74(3)	57(3)	7(2)	-16(2)	10(2)
$C^{(037)}$	40(2)	29.5(19)	56(3)	13.8(17)	-11.9(19)	-13.3(17)
$C^{(038)}$	31(2)	72(3)	27(2)	-11.2(19)	-4.9(17)	12(2)
$C^{(039)}$	85(4)	60(3)	30(2)	7.8(19)	-25(2)	-32(3)
$C^{(03A)}$	34(2)	26.1(18)	40(2)	1.7(15)	-0.8(17)	1.0(16)
$C^{(03B)}$	41(2)	17.5(16)	33.1(19)	5.0(14)	-8.5(16)	-2.4(15)
$C^{(03C)}$	38(2)	28.5(19)	44(2)	1.1(16)	-3.4(18)	9.0(17)
$C^{(03D)}$	34(2)	58(3)	39(2)	17.9(19)	-5.1(18)	6(2)
$C^{(03E)}$	29(2)	52(2)	47(2)	-10.6(19)	-15.2(18)	7.1(18)
$C^{(03F)}$	40(2)	38(2)	34(2)	3.5(16)	-16.6(17)	-7.9(17)
$C^{(03G)}$	35(2)	31.7(19)	30.4(19)	2.9(15)	-6.5(16)	-7.7(16)
$C^{(03H)}$	30.0(19)	23.4(16)	23.2(17)	0.5(13)	-2.1(14)	-7.3(14)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for first_25. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
$C^{(03I)}$	50(3)	53(2)	29(2)	6.8(18)	0.6(18)	-16(2)
$C^{(03L)}$	41(3)	67(3)	52(3)	-1(2)	-3(2)	-30(2)
$C^{(03M)}$	32(2)	26.2(18)	48(2)	-0.1(16)	-9.1(17)	-3.5(16)
$C^{(03N)}$	57(3)	43(2)	28.2(19)	7.0(16)	-16.9(18)	-23(2)
$C^{(03O)}$	27(2)	46(2)	61(3)	-6(2)	-7.3(19)	-6.2(18)
$C^{(03P)}$	19.5(19)	54(2)	38(2)	5.8(18)	-4.7(16)	-0.6(17)
$C^{(03Q)}$	33(3)	78(3)	57(3)	11(2)	14(2)	4(2)
$C^{(03R)}$	29(2)	47(2)	41(2)	-3.6(18)	-3.6(17)	5.4(18)
$C^{(03S)}$	44(4)	18(3)	38(3)	-5(2)	-20(3)	-8(3)
$C^{(03T)}$	28(2)	45(2)	35(2)	-5.6(16)	-3.1(16)	-6.9(17)
$C^{(03V)}$	72(3)	72(3)	38(2)	-10(2)	-23(2)	32(3)
$C^{(03W)}$	30(2)	70(3)	61(3)	-11(2)	-9(2)	14(2)
$C^{(03Z)}$	31(2)	53(2)	46(2)	15.2(19)	3.6(18)	3.0(19)
$C^{(040)}$	30(2)	46(2)	70(3)	-6(2)	3(2)	-15.5(19)
$C^{(041)}$	30(3)	13(2)	28(3)	-3(2)	-6(2)	-0.6(19)
$C^{(042)}$	72(4)	93(4)	35(2)	-12(2)	-27(2)	20(3)
$C^{(043)}$	41(2)	57(3)	45(2)	-1(2)	-16(2)	-14(2)
$C^{(044)}$	59(3)	62(3)	31(2)	6.1(19)	-7.8(19)	-22(2)
$C^{(046)}$	32(2)	33.8(19)	42(2)	8.2(16)	-7.3(17)	-6.8(17)
$C^{(047)}$	43(4)	26(3)	31(3)	4(2)	-22(3)	-4(3)
$C^{(049)}$	45(3)	50(2)	26.4(19)	-8.0(17)	-3.9(17)	9.8(19)
$C^{(04B)}$	30(2)	40(2)	42(2)	-2.0(17)	-2.0(17)	6.3(17)
$C^{(04C)}$	60(3)	23.6(19)	72(3)	0.8(19)	7(2)	-19.2(19)
$C^{(04D)}$	42(3)	43(2)	62(3)	18(2)	-3(2)	-17(2)
$C^{(04E)}$	25(2)	95(4)	66(3)	-6(3)	-11(2)	-12(2)
$C^{(04F)}$	49(3)	45(2)	19.7(17)	-3.8(15)	4.1(16)	-16.1(19)
$C^{(04H)}$	57(4)	22(2)	35(3)	-1(2)	-19(3)	-11(2)
$C^{(8)}$	54(3)	35(2)	35(2)	-1.6(16)	5.6(19)	-11.2(19)
$C^{(10)}$	80(4)	132(5)	47(3)	-53(3)	-21(3)	46(4)
$F^{(1)}$	44.0(14)	52.4(14)	40.4(13)	-4.0(10)	3.1(10)	-12.4(11)
$C^{(4)}$	27(2)	45(2)	30.2(19)	2.2(16)	-5.4(15)	-7.8(17)
$C^{(9)}$	32(2)	74(3)	32(2)	6(2)	0.8(17)	-11(2)
$C^{(1)}$	63(3)	50(2)	26.5(19)	-1.1(17)	-11.2(19)	-27(2)
$C^{(0AA)}$	93(4)	52(3)	38(2)	-2(2)	21(2)	-20(3)
$C^{(1AA)}$	81(4)	59(3)	80(4)	-12(3)	1(3)	-17(3)
$C^{(3)}$	100(4)	55(3)	60(3)	5(2)	3(3)	-32(3)
$C^{(3AA)}$	92(4)	66(3)	82(4)	18(3)	-31(3)	-23(3)
$S^{(4AA)}$	48(3)	19(2)	40(3)	5.4(17)	-9.7(18)	-3.3(16)
$C^{(2)}$	56(4)	18(3)	56(4)	15(3)	-26(3)	-5(2)

Table 4 Bond Lengths for first_25.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
$Ag^{(01)}$	$P^{(005)}$	2.5168(9)	$C^{(01E)}$	$C^{(03D)}$	1.384(5)
$Ag^{(01)}$	$P^{(006)}$	2.4857(8)	$C^{(01F)}$	$C^{(025)}$	1.374(5)
$Ag^{(01)}$	$P^{(007)}$	2.5585(9)	$C^{(01F)}$	$C^{(02K)}$	1.391(5)
$Ag^{(01)}$	$P^{(009)}$	2.5223(8)	$C^{(01G)}$	$C^{(01M)}$	1.389(4)
$Ag^{(02)}$	$P^{(003)}$	2.5014(8)	$C^{(01G)}$	$C^{(025)}$	1.403(4)
$Ag^{(02)}$	$P^{(004)}$	2.4954(8)	$C^{(01H)}$	$C^{(01R)}$	1.385(4)
$Ag^{(02)}$	$P^{(008)}$	2.4546(8)	$C^{(01H)}$	$C^{(02V)}$	1.402(5)
$Ag^{(02)}$	$P^{(00B)}$	2.5477(9)	$C^{(01I)}$	$C^{(029)}$	1.398(5)
$P^{(003)}$	$N^{(00M)}$	1.718(2)	$C^{(01I)}$	$C^{(02X)}$	1.390(4)
$P^{(003)}$	$C^{(00P)}$	1.821(3)	$C^{(01J)}$	$C^{(027)}$	1.387(5)
$P^{(003)}$	$C^{(01G)}$	1.817(3)	$C^{(01K)}$	$C^{(02Y)}$	1.376(5)
$P^{(004)}$	$N^{(00M)}$	1.722(3)	$C^{(01L)}$	$C^{(043)}$	1.364(6)
$P^{(004)}$	$C^{(00W)}$	1.804(3)	$C^{(01M)}$	$C^{(02D)}$	1.388(5)
$P^{(004)}$	$C^{(01E)}$	1.821(3)	$C^{(01O)}$	$C^{(01X)}$	1.389(4)
$P^{(005)}$	$C^{(00L)}$	1.808(3)	$C^{(01O)}$	$C^{(030)}$	1.378(4)
$P^{(005)}$	$C^{(00Z)}$	1.818(3)	$C^{(01P)}$	$C^{(02G)}$	1.392(4)
$P^{(005)}$	$N^{(018)}$	1.729(3)	$C^{(01P)}$	$C^{(02V)}$	1.391(5)

Table 4 Bond Lengths for first_25.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P(006)	C(00S)	1.813(3)	C(01Q)	C(01T)	1.386(4)
P(006)	N(017)	1.713(3)	C(01S)	C(03H)	1.390(5)
P(006)	C(01Y)	1.815(3)	C(01T)	C(022)	1.390(4)
P(007)	N(017)	1.716(3)	C(01W)	C(03F)	1.373(5)
P(007)	C(01B)	1.815(3)	C(01W)	C(04F)	1.382(5)
P(007)	C(03H)	1.828(3)	C(01X)	C(02O)	1.392(4)
P(008)	N(00J)	1.719(3)	C(01Y)	C(02N)	1.396(4)
P(008)	C(00T)	1.814(3)	C(01Y)	C(02R)	1.395(4)
P(008)	C(01I)	1.815(3)	C(01Z)	C(023)	1.387(5)
P(009)	C(014)	1.812(3)	C(01Z)	C(03W)	1.371(6)
P(009)	N(018)	1.717(2)	O(020)	C(02S)	1.415(5)
P(009)	C(019)	1.819(3)	O(020)	C(3)	1.414(5)
S(00A)	C(00V)	1.767(3)	C(021)	C(036)	1.378(5)
S(00A)	C(02H)	1.800(4)	C(024)	C(02R)	1.382(5)
P(00B)	N(00J)	1.735(3)	C(024)	C(03P)	1.367(5)
P(00B)	C(00O)	1.823(3)	C(026)	C(02L)	1.453(7)
P(00B)	C(033)	1.820(3)	C(026)	C(03S)	1.344(6)
S(00C)	C(01C)	1.765(3)	C(026)	C(5)	1.501(16)
S(00C)	C(04C)	1.793(4)	C(026)	C(3BA)	1.17(2)
P(00D)	F(00I)	1.604(2)	C(029)	C(03F)	1.382(5)
P(00D)	F(00K)	1.594(2)	C(02A)	C(038)	1.383(6)
P(00D)	F(00Q)	1.591(2)	C(02B)	C(02Q)	1.385(5)
P(00D)	F(012)	1.600(2)	C(02B)	C(034)	1.380(6)
P(00D)	F(015)	1.605(2)	C(02D)	C(02K)	1.383(5)
P(00D)	F(1)	1.600(2)	C(02E)	C(03L)	1.388(5)
S(00E)	C(02V)	1.755(3)	C(02F)	C(02W)	1.371(6)
S(00E)	C(037)	1.792(4)	C(02F)	C(031)	1.381(6)
S(00F)	C(041)	1.764(5)	C(02I)	C(02W)	1.401(5)
S(00F)	C(2)	1.796(6)	C(02J)	C(03E)	1.378(5)
P(00G)	F(00U)	1.597(3)	C(02L)	C(04H)	1.366(7)
P(00G)	F(013)	1.590(3)	C(02M)	C(049)	1.392(5)
P(00G)	F(01U)	1.603(3)	C(02N)	C(04B)	1.381(5)
P(00G)	F(01V)	1.555(3)	C(02O)	C(03B)	1.392(4)
P(00G)	F(028)	1.588(3)	C(02P)	C(044)	1.368(6)
P(00G)	F(032)	1.578(3)	C(02S)	C(1AA)	1.507(6)
N(00J)	C(01X)	1.435(4)	C(02T)	C(039)	1.384(6)
C(00L)	C(023)	1.390(5)	C(02T)	C(03I)	1.380(6)
C(00L)	C(03Z)	1.388(5)	C(02U)	C(10)	1.393(6)
N(00M)	C(01Q)	1.449(3)	C(02X)	C(04F)	1.388(5)
C(00N)	N(018)	1.445(4)	C(02Y)	C(040)	1.373(6)
C(00N)	C(01R)	1.396(4)	C(02Z)	C(03E)	1.394(5)
C(00N)	C(02G)	1.399(4)	C(02Z)	C(049)	1.369(5)
C(00O)	C(010)	1.374(5)	C(031)	C(03D)	1.384(6)
C(00O)	C(02U)	1.379(5)	C(033)	C(03A)	1.400(4)
C(00P)	C(00X)	1.399(4)	C(033)	C(03M)	1.389(5)
C(00P)	C(4)	1.394(5)	C(034)	C(0AA)	1.364(6)
C(00R)	C(00Y)	1.396(4)	C(036)	C(04E)	1.378(6)
C(00R)	C(01C)	1.377(5)	C(038)	C(9)	1.381(6)
C(00S)	C(02J)	1.390(5)	C(039)	C(03N)	1.383(5)
C(00S)	C(02M)	1.386(5)	C(03A)	C(03C)	1.381(5)
C(00T)	C(021)	1.395(5)	C(03C)	C(03R)	1.380(5)
C(00T)	C(02E)	1.392(5)	C(03G)	C(03I)	1.383(5)
C(00V)	C(030)	1.397(5)	C(03H)	C(03T)	1.394(5)
C(00V)	C(03B)	1.382(5)	C(03L)	C(04E)	1.371(6)
C(00W)	C(03G)	1.383(5)	C(03M)	C(03O)	1.379(5)
C(00W)	C(03N)	1.396(5)	C(03O)	C(03R)	1.378(5)
C(00X)	C(02A)	1.385(5)	C(03P)	C(04B)	1.395(5)
C(00Y)	C(01Q)	1.393(4)	C(03Q)	C(03W)	1.378(6)
C(00Z)	C(02C)	1.387(5)	C(03Q)	C(03Z)	1.375(6)
C(00Z)	C(1)	1.387(5)	C(03S)	C(047)	1.395(8)
C(010)	C(03V)	1.373(5)	C(03T)	C(043)	1.389(5)

Table 4 Bond Lengths for first_25.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C(011)	C(02C)	1.386(5)	C(03V)	C(042)	1.361(6)
C(011)	C(02P)	1.379(6)	C(040)	C(04D)	1.383(6)
C(014)	C(02Q)	1.393(4)	C(041)	C(047)	1.378(7)
C(014)	C(8)	1.385(5)	C(041)	C(04H)	1.374(8)
C(016)	C(019)	1.403(4)	C(042)	C(10)	1.362(7)
C(016)	C(027)	1.381(5)	C(044)	C(1)	1.391(5)
N(017)	C(026)	1.455(4)	C(046)	C(04D)	1.387(5)
C(019)	C(01N)	1.390(4)	C(8)	C(0AA)	1.381(5)
C(01A)	C(01J)	1.387(5)	C(4)	C(9)	1.389(5)
C(01A)	C(01N)	1.390(5)	C(3)	C(3AA)	1.465(7)
C(01B)	C(01K)	1.391(5)	S(4AA)	C(1BA)	1.797(17)
C(01B)	C(046)	1.384(5)	S(4AA)	C(4AA)	1.785(16)
C(01C)	C(022)	1.393(5)	C(2BA)	C(1BA)	1.33(2)
C(01D)	C(01L)	1.383(6)	C(2BA)	C(3BA)	1.43(3)
C(01D)	C(01S)	1.395(5)	C(1BA)	C(0BA)	1.40(2)
C(01E)	C(02I)	1.379(5)	C(0BA)	C(5)	1.42(2)

Table 5 Bond Angles for first_25.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
P(005)	Ag(01)	P(007)	145.79(3)	C(01N)	C(019)	C(016)	118.2(3)
P(005)	Ag(01)	P(009)	67.99(3)	C(01J)	C(01A)	C(01N)	120.7(3)
P(006)	Ag(01)	P(005)	129.93(3)	C(01K)	C(01B)	P(007)	116.8(2)
P(006)	Ag(01)	P(007)	67.90(3)	C(046)	C(01B)	P(007)	123.8(3)
P(006)	Ag(01)	P(009)	128.48(3)	C(046)	C(01B)	C(01K)	119.1(3)
P(009)	Ag(01)	P(007)	128.32(3)	C(00R)	C(01C)	S(00C)	124.3(3)
P(003)	Ag(02)	P(00B)	137.77(3)	C(00R)	C(01C)	C(022)	119.5(3)
P(004)	Ag(02)	P(003)	68.73(3)	C(022)	C(01C)	S(00C)	116.2(2)
P(004)	Ag(02)	P(00B)	128.57(3)	C(01L)	C(01D)	C(01S)	119.7(4)
P(008)	Ag(02)	P(003)	133.11(3)	C(02I)	C(01E)	P(004)	116.9(3)
P(008)	Ag(02)	P(004)	132.15(3)	C(02I)	C(01E)	C(03D)	118.7(3)
P(008)	Ag(02)	P(00B)	68.75(3)	C(03D)	C(01E)	P(004)	124.3(3)
N(00M)	P(003)	Ag(02)	90.21(8)	C(025)	C(01F)	C(02K)	120.1(3)
N(00M)	P(003)	C(00P)	106.54(13)	C(01M)	C(01G)	P(003)	124.9(2)
N(00M)	P(003)	C(01G)	106.37(13)	C(01M)	C(01G)	C(025)	118.9(3)
C(00P)	P(003)	Ag(02)	121.26(11)	C(025)	C(01G)	P(003)	115.6(2)
C(01G)	P(003)	Ag(02)	122.10(10)	C(01R)	C(01H)	C(02V)	121.8(3)
C(01G)	P(003)	C(00P)	106.60(14)	C(029)	C(01I)	P(008)	118.0(2)
N(00M)	P(004)	Ag(02)	90.32(8)	C(02X)	C(01I)	P(008)	121.8(3)
N(00M)	P(004)	C(00W)	107.50(14)	C(02X)	C(01I)	C(029)	118.6(3)
N(00M)	P(004)	C(01E)	106.60(13)	C(01A)	C(01J)	C(027)	119.2(3)
C(00W)	P(004)	Ag(02)	120.46(11)	C(02Y)	C(01K)	C(01B)	120.4(3)
C(00W)	P(004)	C(01E)	105.36(15)	C(043)	C(01L)	C(01D)	120.3(4)
C(01E)	P(004)	Ag(02)	123.43(10)	C(01G)	C(01M)	C(02D)	120.1(3)
C(00L)	P(005)	Ag(01)	125.44(11)	C(019)	C(01N)	C(01A)	120.5(3)
C(00L)	P(005)	C(00Z)	104.37(15)	C(030)	C(01O)	C(01X)	120.6(3)
C(00Z)	P(005)	Ag(01)	119.41(11)	C(02V)	C(01P)	C(02G)	120.7(3)
N(018)	P(005)	Ag(01)	90.98(9)	C(00Y)	C(01Q)	N(00M)	120.2(3)
N(018)	P(005)	C(00L)	105.47(14)	C(01T)	C(01Q)	N(00M)	120.3(3)
N(018)	P(005)	C(00Z)	108.10(14)	C(01T)	C(01Q)	C(00Y)	119.6(3)
C(00S)	P(006)	Ag(01)	116.44(10)	C(01H)	C(01R)	C(00N)	120.5(3)
C(00S)	P(006)	C(01Y)	105.63(15)	C(03H)	C(01S)	C(01D)	120.4(4)
N(017)	P(006)	Ag(01)	92.05(9)	C(01Q)	C(01T)	C(022)	119.7(3)
N(017)	P(006)	C(00S)	107.92(14)	C(03F)	C(01W)	C(04F)	119.7(3)
N(017)	P(006)	C(01Y)	107.11(14)	C(01O)	C(01X)	N(00J)	120.9(3)
C(01Y)	P(006)	Ag(01)	125.28(11)	C(01O)	C(01X)	C(02O)	118.7(3)
N(017)	P(007)	Ag(01)	89.51(9)	C(02O)	C(01X)	N(00J)	120.4(3)
N(017)	P(007)	C(01B)	102.98(14)	C(02N)	C(01Y)	P(006)	124.7(3)
N(017)	P(007)	C(03H)	107.73(14)	C(02R)	C(01Y)	P(006)	116.4(2)
C(01B)	P(007)	Ag(01)	135.08(11)	C(02R)	C(01Y)	C(02N)	118.9(3)
C(01B)	P(007)	C(03H)	105.17(15)	C(03W)	C(01Z)	C(023)	120.7(4)

Table 5 Bond Angles for first_25.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(03H)	P(007)	Ag(01)	111.74(10)	C(3)	O(020)	C(02S)	113.1(4)
N(00J)	P(008)	Ag(02)	92.37(9)	C(036)	C(021)	C(00T)	120.4(4)
N(00J)	P(008)	C(00T)	107.62(14)	C(01T)	C(022)	C(01C)	120.7(3)
N(00J)	P(008)	C(01I)	108.71(13)	C(01Z)	C(023)	C(00L)	120.0(4)
C(00T)	P(008)	Ag(02)	122.13(11)	C(03P)	C(024)	C(02R)	119.4(3)
C(00T)	P(008)	C(01I)	107.05(15)	C(01F)	C(025)	C(01G)	120.7(3)
C(01I)	P(008)	Ag(02)	116.94(10)	N(017)	C(026)	C(5)	109.4(6)
C(014)	P(009)	Ag(01)	118.83(11)	C(02L)	C(026)	N(017)	118.4(3)
C(014)	P(009)	C(019)	106.02(14)	C(03S)	C(026)	N(017)	125.9(4)
N(018)	P(009)	Ag(01)	91.06(9)	C(03S)	C(026)	C(02L)	115.7(4)
N(018)	P(009)	C(014)	108.46(14)	C(3BA)	C(026)	N(017)	125.5(10)
N(018)	P(009)	C(019)	105.17(13)	C(3BA)	C(026)	C(5)	124.2(12)
C(019)	P(009)	Ag(01)	124.17(10)	C(016)	C(027)	C(01J)	120.2(3)
C(00V)	S(00A)	C(02H)	103.26(17)	C(03F)	C(029)	C(01I)	120.6(3)
N(00J)	P(00B)	Ag(02)	88.89(9)	C(038)	C(02A)	C(00X)	119.9(4)
N(00J)	P(00B)	C(00O)	108.32(14)	C(034)	C(02B)	C(02Q)	119.8(3)
N(00J)	P(00B)	C(033)	108.21(14)	C(011)	C(02C)	C(00Z)	120.2(4)
C(00O)	P(00B)	Ag(02)	116.47(11)	C(02K)	C(02D)	C(01M)	120.6(3)
C(033)	P(00B)	Ag(02)	129.88(11)	C(03L)	C(02E)	C(00T)	119.7(4)
C(033)	P(00B)	C(00O)	102.51(15)	C(02W)	C(02F)	C(031)	118.9(4)
C(01C)	S(00C)	C(04C)	103.93(17)	C(01P)	C(02G)	C(00N)	121.4(3)
F(00I)	P(00D)	F(015)	178.46(14)	C(01E)	C(02I)	C(02W)	120.4(3)
F(00K)	P(00D)	F(00I)	89.86(13)	C(03E)	C(02J)	C(00S)	121.4(3)
F(00K)	P(00D)	F(012)	90.33(13)	C(02D)	C(02K)	C(01F)	119.6(3)
F(00K)	P(00D)	F(015)	88.61(13)	C(04H)	C(02L)	C(026)	120.9(5)
F(00K)	P(00D)	F(1)	89.34(12)	C(00S)	C(02M)	C(049)	120.0(3)
F(00Q)	P(00D)	F(00I)	91.18(15)	C(04B)	C(02N)	C(01Y)	119.9(3)
F(00Q)	P(00D)	F(00K)	178.93(17)	C(03B)	C(02O)	C(01X)	120.5(3)
F(00Q)	P(00D)	F(012)	89.44(14)	C(044)	C(02P)	C(011)	119.5(4)
F(00Q)	P(00D)	F(015)	90.36(15)	C(02B)	C(02Q)	C(014)	119.7(3)
F(00Q)	P(00D)	F(1)	90.90(14)	C(024)	C(02R)	C(01Y)	121.0(3)
F(012)	P(00D)	F(00I)	89.43(13)	O(020)	C(02S)	C(1AA)	109.1(4)
F(012)	P(00D)	F(015)	90.60(13)	C(03I)	C(02T)	C(039)	119.8(4)
F(012)	P(00D)	F(1)	179.66(15)	C(00O)	C(02U)	C(10)	120.4(4)
F(1)	P(00D)	F(00I)	90.52(13)	C(01H)	C(02V)	S(00E)	117.0(3)
F(1)	P(00D)	F(015)	89.45(13)	C(01P)	C(02V)	S(00E)	125.3(3)
C(02V)	S(00E)	C(037)	103.17(17)	C(01P)	C(02V)	C(01H)	117.7(3)
C(041)	S(00F)	C(2)	103.5(3)	C(02F)	C(02W)	C(02I)	120.6(4)
F(00U)	P(00G)	F(01U)	88.91(19)	C(04F)	C(02X)	C(01I)	120.1(3)
F(013)	P(00G)	F(00U)	178.62(19)	C(040)	C(02Y)	C(01K)	120.0(4)
F(013)	P(00G)	F(01U)	89.80(17)	C(049)	C(02Z)	C(03E)	119.9(4)
F(01V)	P(00G)	F(00U)	90.7(2)	C(01O)	C(030)	C(00V)	120.9(3)
F(01V)	P(00G)	F(013)	90.52(18)	C(02F)	C(031)	C(03D)	120.8(4)
F(01V)	P(00G)	F(01U)	176.6(2)	C(03A)	C(033)	P(00B)	125.8(3)
F(01V)	P(00G)	F(028)	88.7(2)	C(03M)	C(033)	P(00B)	116.1(2)
F(01V)	P(00G)	F(032)	93.5(2)	C(03M)	C(033)	C(03A)	118.0(3)
F(028)	P(00G)	F(00U)	88.52(17)	C(0AA)	C(034)	C(02B)	120.9(4)
F(028)	P(00G)	F(013)	90.96(16)	C(04E)	C(036)	C(021)	119.8(4)
F(028)	P(00G)	F(01U)	87.9(2)	C(9)	C(038)	C(02A)	120.5(3)
F(032)	P(00G)	F(00U)	90.94(17)	C(03N)	C(039)	C(02T)	120.3(4)
F(032)	P(00G)	F(013)	89.53(17)	C(03C)	C(03A)	C(033)	120.4(3)
F(032)	P(00G)	F(01U)	89.9(2)	C(00V)	C(03B)	C(02O)	120.6(3)
F(032)	P(00G)	F(028)	177.8(2)	C(03R)	C(03C)	C(03A)	120.6(3)
P(008)	N(00J)	P(00B)	109.79(13)	C(01E)	C(03D)	C(031)	120.6(4)
C(01X)	N(00J)	P(008)	123.8(2)	C(02J)	C(03E)	C(02Z)	119.2(4)
C(01X)	N(00J)	P(00B)	125.4(2)	C(01W)	C(03F)	C(029)	120.3(4)
C(023)	C(00L)	P(005)	124.2(3)	C(00W)	C(03G)	C(03I)	120.1(3)
C(03Z)	C(00L)	P(005)	116.9(3)	C(01S)	C(03H)	P(007)	119.4(3)
C(03Z)	C(00L)	C(023)	118.8(3)	C(01S)	C(03H)	C(03T)	118.9(3)
P(003)	N(00M)	P(004)	110.18(13)	C(03T)	C(03H)	P(007)	120.8(3)
C(01Q)	N(00M)	P(003)	124.6(2)	C(02T)	C(03I)	C(03G)	120.4(4)

Table 5 Bond Angles for first_25.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C(01Q)	N(00M)	P(004)	124.7(2)	C(04E)	C(03L)	C(02E)	120.2(4)
C(01R)	C(00N)	N(018)	121.6(3)	C(03O)	C(03M)	C(033)	121.3(3)
C(01R)	C(00N)	C(02G)	117.9(3)	C(039)	C(03N)	C(00W)	119.7(4)
C(02G)	C(00N)	N(018)	120.4(3)	C(03R)	C(03O)	C(03M)	120.1(4)
C(010)	C(00O)	P(00B)	118.9(3)	C(024)	C(03P)	C(04B)	120.7(3)
C(010)	C(00O)	C(02U)	117.6(3)	C(03Z)	C(03Q)	C(03W)	120.5(4)
C(02U)	C(00O)	P(00B)	123.4(3)	C(03O)	C(03R)	C(03C)	119.6(4)
C(00X)	C(00P)	P(003)	124.4(3)	C(026)	C(03S)	C(047)	123.0(5)
C(4)	C(00P)	P(003)	116.5(3)	C(043)	C(03T)	C(03H)	120.0(3)
C(4)	C(00P)	C(00X)	119.1(3)	C(042)	C(03V)	C(010)	119.8(4)
C(01C)	C(00R)	C(00Y)	120.1(3)	C(01Z)	C(03W)	C(03Q)	119.5(4)
C(02J)	C(00S)	P(006)	117.3(2)	C(03Q)	C(03Z)	C(00L)	120.5(4)
C(02M)	C(00S)	P(006)	123.7(3)	C(02Y)	C(040)	C(04D)	120.6(4)
C(02M)	C(00S)	C(02J)	118.7(3)	C(047)	C(041)	S(00F)	125.3(5)
C(021)	C(00T)	P(008)	116.4(3)	C(04H)	C(041)	S(00F)	116.3(4)
C(02E)	C(00T)	P(008)	124.3(3)	C(04H)	C(041)	C(047)	118.3(4)
C(02E)	C(00T)	C(021)	119.2(3)	C(03V)	C(042)	C(10)	119.7(4)
C(030)	C(00V)	S(00A)	116.7(3)	C(01L)	C(043)	C(03T)	120.6(4)
C(03B)	C(00V)	S(00A)	124.8(3)	C(02P)	C(044)	C(1)	120.5(4)
C(03B)	C(00V)	C(030)	118.6(3)	C(01B)	C(046)	C(04D)	120.5(4)
C(03G)	C(00W)	P(004)	122.1(3)	C(041)	C(047)	C(03S)	120.6(5)
C(03G)	C(00W)	C(03N)	119.7(3)	C(02Z)	C(049)	C(02M)	120.7(3)
C(03N)	C(00W)	P(004)	117.5(3)	C(02N)	C(04B)	C(03P)	120.0(3)
C(02A)	C(00X)	C(00P)	120.3(3)	C(040)	C(04D)	C(046)	119.3(4)
C(01Q)	C(00Y)	C(00R)	120.3(3)	C(03L)	C(04E)	C(036)	120.6(4)
C(02C)	C(00Z)	P(005)	115.3(3)	C(01W)	C(04F)	C(02X)	120.5(3)
C(02C)	C(00Z)	C(1)	118.9(3)	C(02L)	C(04H)	C(041)	121.4(5)
C(1)	C(00Z)	P(005)	125.8(3)	C(0AA)	C(8)	C(014)	120.8(4)
C(03V)	C(010)	C(00O)	122.0(4)	C(042)	C(10)	C(02U)	120.4(4)
C(02P)	C(011)	C(02C)	120.6(4)	C(9)	C(4)	C(00P)	120.3(4)
C(02Q)	C(014)	P(009)	125.5(2)	C(038)	C(9)	C(4)	119.9(4)
C(8)	C(014)	P(009)	115.4(2)	C(00Z)	C(1)	C(044)	120.3(3)
C(8)	C(014)	C(02Q)	119.1(3)	C(034)	C(0AA)	C(8)	119.6(4)
C(027)	C(016)	C(019)	121.1(3)	O(020)	C(3)	C(3AA)	109.7(4)
P(006)	N(017)	P(007)	110.53(14)	C(4AA)	S(4AA)	C(1BA)	99.9(12)
C(026)	N(017)	P(006)	125.0(2)	C(1BA)	C(2BA)	C(3BA)	119.1(17)
C(026)	N(017)	P(007)	124.4(2)	C(2BA)	C(1BA)	S(4AA)	126.8(17)
P(009)	N(018)	P(005)	109.69(13)	C(2BA)	C(1BA)	C(0BA)	121.9(16)
C(00N)	N(018)	P(005)	126.6(2)	C(0BA)	C(1BA)	S(4AA)	111.3(13)
C(00N)	N(018)	P(009)	122.7(2)	C(1BA)	C(0BA)	C(5)	117.7(15)
C(016)	C(019)	P(009)	117.6(2)	C(0BA)	C(5)	C(026)	114.9(12)
C(01N)	C(019)	P(009)	123.8(2)	C(026)	C(3BA)	C(2BA)	121.4(18)

Table 6 Torsion Angles for first_25.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ag(01)	P(005)	C(00L)	C(023)	-162.2(2)	N(017)	P(007)	C(03H)	C(01S)	-158.4(3)
Ag(01)	P(005)	C(00L)	C(03Z)	22.0(3)	N(017)	P(007)	C(03H)	C(03T)	31.9(3)
Ag(01)	P(005)	C(00Z)	C(02C)	60.8(3)	N(017)	C(026)	C(02L)	C(04H)	179.6(5)
Ag(01)	P(005)	C(00Z)	C(1)	-117.6(3)	N(017)	C(026)	C(03S)	C(047)	179.0(5)
Ag(01)	P(005)	N(018)	P(009)	-4.85(13)	N(017)	C(026)	C(5)	C(0BA)	177.7(10)
Ag(01)	P(005)	N(018)	C(00N)	-174.0(2)	N(017)	C(026)	C(3BA)	C(2BA)	-178.8(11)
Ag(01)	P(006)	C(00S)	C(02J)	-45.3(3)	N(018)	P(005)	C(00L)	C(023)	95.2(3)
Ag(01)	P(006)	C(00S)	C(02M)	128.0(3)	N(018)	P(005)	C(00L)	C(03Z)	-80.7(3)
Ag(01)	P(006)	N(017)	P(007)	-0.83(14)	N(018)	P(005)	C(00Z)	C(02C)	162.7(3)
Ag(01)	P(006)	N(017)	C(026)	174.9(2)	N(018)	P(005)	C(00Z)	C(1)	-15.7(4)
Ag(01)	P(006)	C(01Y)	C(02N)	163.2(2)	N(018)	P(009)	C(014)	C(02Q)	-58.5(3)
Ag(01)	P(006)	C(01Y)	C(02R)	-17.9(3)	N(018)	P(009)	C(014)	C(8)	121.6(3)
Ag(01)	P(007)	N(017)	P(006)	0.80(13)	N(018)	P(009)	C(019)	C(016)	-56.7(3)
Ag(01)	P(007)	N(017)	C(026)	-174.9(2)	N(018)	P(009)	C(019)	C(01N)	130.6(3)
Ag(01)	P(007)	C(01B)	C(01K)	13.5(3)	N(018)	C(00N)	C(01R)	C(01H)	179.9(3)

Table 6 Torsion Angles for first_25.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ag(01)	P(007)	C(01B)	C(046)	-172.6(2)	N(018)	C(00N)	C(02G)	C(01P)	-177.6(3)
Ag(01)	P(007)	C(03H)	C(01S)	104.8(3)	C(019)	P(009)	C(014)	C(02Q)	54.0(3)
Ag(01)	P(007)	C(03H)	C(03T)	-64.8(3)	C(019)	P(009)	C(014)	C(8)	-125.9(3)
Ag(01)	P(009)	C(014)	C(02Q)	-160.4(2)	C(019)	P(009)	N(018)	P(005)	130.79(15)
Ag(01)	P(009)	C(014)	C(8)	19.7(3)	C(019)	P(009)	N(018)	C(00N)	-59.6(3)
Ag(01)	P(009)	N(018)	P(005)	4.84(13)	C(019)	C(016)	C(027)	C(01J)	0.7(5)
Ag(01)	P(009)	N(018)	C(00N)	174.5(2)	C(01A)	C(01J)	C(027)	C(016)	-0.4(5)
Ag(01)	P(009)	C(019)	C(016)	45.3(3)	C(01B)	P(007)	N(017)	P(006)	137.25(16)
Ag(01)	P(009)	C(019)	C(01N)	-127.4(2)	C(01B)	P(007)	N(017)	C(026)	-38.5(3)
Ag(02)	P(003)	N(00M)	P(004)	6.81(13)	C(01B)	P(007)	C(03H)	C(01S)	-49.1(3)
Ag(02)	P(003)	N(00M)	C(01Q)	178.8(2)	C(01B)	P(007)	C(03H)	C(03T)	141.3(3)
Ag(02)	P(003)	C(00P)	C(00X)	-158.3(2)	C(01B)	C(01K)	C(02Y)	C(040)	1.2(6)
Ag(02)	P(003)	C(00P)	C(4)	19.1(3)	C(01B)	C(046)	C(04D)	C(040)	2.6(6)
Ag(02)	P(003)	C(01G)	C(01M)	-135.6(2)	C(01C)	C(00R)	C(00Y)	C(01Q)	-1.1(5)
Ag(02)	P(003)	C(01G)	C(025)	35.7(3)	C(01D)	C(01L)	C(043)	C(03T)	0.5(6)
Ag(02)	P(004)	N(00M)	P(003)	-6.83(13)	C(01D)	C(01S)	C(03H)	P(007)	-170.6(3)
Ag(02)	P(004)	N(00M)	C(01Q)	-178.8(2)	C(01D)	C(01S)	C(03H)	C(03T)	-0.7(5)
Ag(02)	P(004)	C(00W)	C(03G)	-80.4(3)	C(01E)	P(004)	N(00M)	P(003)	118.37(16)
Ag(02)	P(004)	C(00W)	C(03N)	89.7(3)	C(01E)	P(004)	N(00M)	C(01Q)	-53.6(3)
Ag(02)	P(004)	C(01E)	C(02I)	23.4(3)	C(01E)	P(004)	C(00W)	C(03G)	134.1(3)
Ag(02)	P(004)	C(01E)	C(03D)	-160.4(3)	C(01E)	P(004)	C(00W)	C(03N)	-55.8(3)
Ag(02)	P(008)	N(00J)	P(00B)	-4.08(13)	C(01E)	C(02I)	C(02W)	C(02F)	1.2(7)
Ag(02)	P(008)	N(00J)	C(01X)	-173.6(2)	C(01G)	P(003)	N(00M)	P(004)	130.52(15)
Ag(02)	P(008)	C(00T)	C(021)	1.3(3)	C(01G)	P(003)	N(00M)	C(01Q)	-57.5(3)
Ag(02)	P(008)	C(00T)	C(02E)	-176.5(2)	C(01G)	P(003)	C(00P)	C(00X)	55.6(3)
Ag(02)	P(008)	C(01I)	C(029)	-55.5(3)	C(01G)	P(003)	C(00P)	C(4)	-127.0(3)
Ag(02)	P(008)	C(01I)	C(02X)	109.9(2)	C(01G)	C(01M)	C(02D)	C(02K)	0.5(5)
Ag(02)	P(00B)	N(00J)	P(008)	3.93(13)	C(01I)	P(008)	N(00J)	P(00B)	-123.60(15)
Ag(02)	P(00B)	N(00J)	C(01X)	173.3(2)	C(01I)	P(008)	N(00J)	C(01X)	66.9(3)
Ag(02)	P(00B)	C(00O)	C(010)	-21.5(3)	C(01I)	P(008)	C(00T)	C(021)	140.0(3)
Ag(02)	P(00B)	C(00O)	C(02U)	156.0(3)	C(01I)	P(008)	C(00T)	C(02E)	-37.7(3)
Ag(02)	P(00B)	C(033)	C(03A)	143.7(3)	C(01I)	C(029)	C(03F)	C(01W)	-0.7(5)
Ag(02)	P(00B)	C(033)	C(03M)	-39.2(3)	C(01I)	C(02X)	C(04F)	C(01W)	0.2(5)
P(003)	N(00M)	C(01Q)	C(00Y)	72.2(3)	C(01J)	C(01A)	C(01N)	C(019)	-0.9(5)
P(003)	N(00M)	C(01Q)	C(01T)	-107.7(3)	C(01K)	C(01B)	C(046)	C(04D)	-0.6(5)
P(003)	C(00P)	C(00X)	C(02A)	177.5(3)	C(01K)	C(02Y)	C(040)	C(04D)	0.8(6)
P(003)	C(00P)	C(4)	C(9)	-177.4(3)	C(01L)	C(01D)	C(01S)	C(03H)	-0.4(5)
P(003)	C(01G)	C(01M)	C(02D)	171.2(3)	C(01M)	C(01G)	C(025)	C(01F)	-0.9(5)
P(003)	C(01G)	C(025)	C(01F)	-172.7(3)	C(01M)	C(02D)	C(02K)	C(01F)	-0.5(6)
P(004)	N(00M)	C(01Q)	C(00Y)	-117.0(3)	C(01N)	C(01A)	C(01J)	C(027)	0.5(5)
P(004)	N(00M)	C(01Q)	C(01T)	63.1(4)	C(01O)	C(01X)	C(02O)	C(03B)	0.8(5)
P(004)	C(00W)	C(03G)	C(03I)	171.3(3)	C(01Q)	C(01T)	C(022)	C(01C)	-1.4(5)
P(004)	C(00W)	C(03N)	C(039)	-171.8(3)	C(01R)	C(00N)	N(018)	P(005)	60.6(4)
P(004)	C(01E)	C(02I)	C(02W)	175.7(3)	C(01R)	C(00N)	N(018)	P(009)	-107.2(3)
P(004)	C(01E)	C(03D)	C(031)	-176.0(3)	C(01R)	C(00N)	C(02G)	C(01P)	0.4(5)
P(005)	C(00L)	C(023)	C(01Z)	-174.3(3)	C(01R)	C(01H)	C(02V)	S(00E)	-178.4(3)
P(005)	C(00L)	C(03Z)	C(03Q)	173.1(4)	C(01R)	C(01H)	C(02V)	C(01P)	1.5(5)
P(005)	C(00Z)	C(02C)	C(011)	-179.5(3)	C(01S)	C(01D)	C(01L)	C(043)	0.5(6)
P(005)	C(00Z)	C(1)	C(044)	178.2(3)	C(01S)	C(03H)	C(03T)	C(043)	1.7(5)
P(006)	C(00S)	C(02J)	C(03E)	175.6(3)	C(01X)	C(01O)	C(030)	C(00V)	0.7(6)
P(006)	C(00S)	C(02M)	C(049)	-174.4(3)	C(01X)	C(02O)	C(03B)	C(00V)	0.8(5)
P(006)	N(017)	C(026)	C(02L)	-59.6(5)	C(01Y)	P(006)	C(00S)	C(02J)	170.7(3)
P(006)	N(017)	C(026)	C(03S)	121.5(4)	C(01Y)	P(006)	C(00S)	C(02M)	-16.0(3)
P(006)	N(017)	C(026)	C(5)	109.8(6)	C(01Y)	P(006)	N(017)	P(007)	127.18(16)
P(006)	N(017)	C(026)	C(3BA)	-80.5(12)	C(01Y)	P(006)	N(017)	C(026)	-57.1(3)
P(006)	C(01Y)	C(02N)	C(04B)	177.6(3)	C(01Y)	C(02N)	C(04B)	C(03P)	-0.4(5)
P(006)	C(01Y)	C(02R)	C(024)	-176.6(3)	C(021)	C(00T)	C(02E)	C(03L)	-0.3(5)
P(007)	N(017)	C(026)	C(02L)	115.5(4)	C(021)	C(036)	C(04E)	C(03L)	-0.5(7)
P(007)	N(017)	C(026)	C(03S)	-63.4(5)	C(023)	C(00L)	C(03Z)	C(03Q)	-3.0(6)
P(007)	N(017)	C(026)	C(5)	-75.1(7)	C(023)	C(01Z)	C(03W)	C(03Q)	-0.6(7)
P(007)	N(017)	C(026)	C(3BA)	94.6(12)	C(024)	C(03P)	C(04B)	C(02N)	1.0(6)

Table 6 Torsion Angles for first_25.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P(007)	C(01B)	C(01K)	C(02Y)	172.9(3)	C(025)	C(01F)	C(02K)	C(02D)	-0.2(5)
P(007)	C(01B)	C(046)	C(04D)	-174.3(3)	C(025)	C(01G)	C(01M)	C(02D)	0.2(5)
P(007)	C(03H)	C(03T)	C(043)	171.4(3)	C(026)	C(02L)	C(04H)	C(041)	0.8(10)
P(008)	N(00J)	C(01X)	C(01O)	107.0(3)	C(026)	C(03S)	C(047)	C(041)	1.9(9)
P(008)	N(00J)	C(01X)	C(02O)	-73.9(4)	C(027)	C(016)	C(019)	P(009)	-174.2(2)
P(008)	C(00T)	C(021)	C(036)	-178.2(3)	C(027)	C(016)	C(019)	C(01N)	-1.0(5)
P(008)	C(00T)	C(02E)	C(03L)	177.4(3)	C(029)	C(01I)	C(02X)	C(04F)	-0.5(5)
P(008)	C(01I)	C(029)	C(03F)	166.6(3)	C(02A)	C(038)	C(9)	C(4)	0.3(6)
P(008)	C(01I)	C(02X)	C(04F)	-165.8(3)	C(02B)	C(034)	C(0AA)	C(8)	0.5(8)
P(009)	C(014)	C(02Q)	C(02B)	180.0(3)	C(02C)	C(00Z)	C(1)	C(044)	-0.2(6)
P(009)	C(014)	C(8)	C(0AA)	180.0(4)	C(02C)	C(011)	C(02P)	C(044)	-0.6(6)
P(009)	C(019)	C(01N)	C(01A)	173.8(3)	C(02E)	C(00T)	C(021)	C(036)	-0.3(5)
S(00A)	C(00V)	C(030)	C(01O)	-180.0(3)	C(02E)	C(03L)	C(04E)	C(036)	-0.1(7)
S(00A)	C(00V)	C(03B)	C(02O)	179.3(3)	C(02F)	C(031)	C(03D)	C(01E)	0.1(7)
P(00B)	N(00J)	C(01X)	C(01O)	-60.9(4)	C(02G)	C(00N)	N(018)	P(005)	-121.4(3)
P(00B)	N(00J)	C(01X)	C(02O)	118.2(3)	C(02G)	C(00N)	N(018)	P(009)	70.8(3)
P(00B)	C(00O)	C(010)	C(03V)	177.6(4)	C(02G)	C(00N)	C(01R)	C(01H)	1.9(5)
P(00B)	C(00O)	C(02U)	C(10)	-176.4(5)	C(02G)	C(01P)	C(02V)	S(00E)	-179.3(3)
P(00B)	C(033)	C(03A)	C(03C)	177.3(3)	C(02G)	C(01P)	C(02V)	C(01H)	0.8(5)
P(00B)	C(033)	C(03M)	C(03O)	-176.3(3)	C(02H)	S(00A)	C(00V)	C(030)	-169.8(3)
S(00C)	C(01C)	C(022)	C(01T)	176.6(2)	C(02H)	S(00A)	C(00V)	C(03B)	9.3(4)
S(00F)	C(041)	C(047)	C(03S)	178.7(4)	C(02I)	C(01E)	C(03D)	C(031)	0.2(6)
S(00F)	C(041)	C(04H)	C(02L)	-179.9(5)	C(02J)	C(00S)	C(02M)	C(049)	-1.2(5)
N(00J)	P(008)	C(00T)	C(021)	-103.2(3)	C(02K)	C(01F)	C(025)	C(01G)	0.9(5)
N(00J)	P(008)	C(00T)	C(02E)	79.0(3)	C(02L)	C(026)	C(03S)	C(047)	0.0(8)
N(00J)	P(008)	C(01I)	C(029)	47.2(3)	C(02M)	C(00S)	C(02J)	C(03E)	2.0(5)
N(00J)	P(008)	C(01I)	C(02X)	-147.3(2)	C(02N)	C(01Y)	C(02R)	C(024)	2.4(5)
N(00J)	P(00B)	C(00O)	C(010)	76.7(3)	C(02P)	C(011)	C(02C)	C(00Z)	1.4(6)
N(00J)	P(00B)	C(00O)	C(02U)	-105.8(4)	C(02P)	C(044)	C(1)	C(00Z)	0.9(7)
N(00J)	P(00B)	C(033)	C(03A)	39.4(3)	C(02Q)	C(014)	C(8)	C(0AA)	0.0(6)
N(00J)	P(00B)	C(033)	C(03M)	-143.6(3)	C(02Q)	C(02B)	C(034)	C(0AA)	-0.6(7)
N(00J)	C(01X)	C(02O)	C(03B)	-178.3(3)	C(02R)	C(01Y)	C(02N)	C(04B)	-1.3(5)
C(00L)	P(005)	C(00Z)	C(02C)	-85.4(3)	C(02R)	C(024)	C(03P)	C(04B)	0.2(5)
C(00L)	P(005)	C(00Z)	C(1)	96.2(3)	C(02S)	O(020)	C(3)	C(3AA)	-174.7(4)
C(00L)	P(005)	N(018)	P(009)	122.48(16)	C(02T)	C(039)	C(03N)	C(00W)	0.5(7)
C(00L)	P(005)	N(018)	C(00N)	-46.7(3)	C(02U)	C(00O)	C(010)	C(03V)	-0.1(7)
N(00M)	P(003)	C(00P)	C(00X)	-57.7(3)	C(02V)	C(01H)	C(01R)	C(00N)	-2.9(5)
N(00M)	P(003)	C(00P)	C(4)	119.7(3)	C(02V)	C(01P)	C(02G)	C(00N)	-1.8(5)
N(00M)	P(003)	C(01G)	C(01M)	123.5(3)	C(02W)	C(02F)	C(031)	C(03D)	0.3(7)
N(00M)	P(003)	C(01G)	C(025)	-65.2(3)	C(02X)	C(01I)	C(029)	C(03F)	0.7(5)
N(00M)	P(004)	C(00W)	C(03G)	20.7(3)	C(02Y)	C(040)	C(04D)	C(046)	-2.7(7)
N(00M)	P(004)	C(00W)	C(03N)	-169.2(3)	C(030)	C(00V)	C(03B)	C(02O)	-1.7(5)
N(00M)	P(004)	C(01E)	C(02I)	-78.4(3)	C(030)	C(01O)	C(01X)	N(00J)	177.6(3)
N(00M)	P(004)	C(01E)	C(03D)	97.9(3)	C(030)	C(01O)	C(01X)	C(02O)	-1.5(5)
N(00M)	C(01Q)	C(01T)	C(022)	-176.4(3)	C(031)	C(02F)	C(02W)	C(02I)	-0.9(7)
C(00O)	P(00B)	N(00J)	P(008)	-113.67(16)	C(033)	P(00B)	N(00J)	P(008)	135.90(15)
C(00O)	P(00B)	N(00J)	C(01X)	55.7(3)	C(033)	P(00B)	N(00J)	C(01X)	-54.8(3)
C(00O)	P(00B)	C(033)	C(03A)	-75.0(3)	C(033)	P(00B)	C(00O)	C(010)	-169.1(3)
C(00O)	P(00B)	C(033)	C(03M)	102.1(3)	C(033)	P(00B)	C(00O)	C(02U)	8.4(4)
C(00O)	C(010)	C(03V)	C(042)	-2.1(8)	C(033)	C(03A)	C(03C)	C(03R)	-1.1(6)
C(00O)	C(02U)	C(10)	C(042)	0.0(10)	C(033)	C(03M)	C(03O)	C(03R)	-1.5(6)
C(00P)	P(003)	N(00M)	P(004)	-116.04(16)	C(034)	C(02B)	C(02Q)	C(014)	0.3(6)
C(00P)	P(003)	N(00M)	C(01Q)	56.0(3)	C(037)	S(00E)	C(02V)	C(01H)	175.5(3)
C(00P)	P(003)	C(01G)	C(01M)	10.1(3)	C(037)	S(00E)	C(02V)	C(01P)	-4.4(3)
C(00P)	P(003)	C(01G)	C(025)	-178.6(2)	C(039)	C(02T)	C(03I)	C(03G)	-0.7(7)
C(00P)	C(00X)	C(02A)	C(038)	-0.2(5)	C(03A)	C(033)	C(03M)	C(03O)	1.0(5)
C(00P)	C(4)	C(9)	C(038)	-0.3(6)	C(03A)	C(03C)	C(03R)	C(03O)	0.6(6)
C(00R)	C(00Y)	C(01Q)	N(00M)	177.7(3)	C(03B)	C(00V)	C(030)	C(01O)	0.9(5)
C(00R)	C(00Y)	C(01Q)	C(01T)	-2.4(5)	C(03D)	C(01E)	C(02I)	C(02W)	-0.8(6)
C(00R)	C(01C)	C(022)	C(01T)	-2.1(5)	C(03E)	C(02Z)	C(049)	C(02M)	2.3(6)
C(00S)	P(006)	N(017)	P(007)	-119.50(16)	C(03F)	C(01W)	C(04F)	C(02X)	-0.2(5)

Table 6 Torsion Angles for first_25.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C(00S)	P(006)	N(017)	C(026)	56.2(3)	C(03G)	C(00W)	C(03N)	C(039)	-1.5(6)
C(00S)	P(006)	C(01Y)	C(02N)	-57.0(3)	C(03H)	P(007)	N(017)	P(006)	-111.92(16)
C(00S)	P(006)	C(01Y)	C(02R)	121.9(3)	C(03H)	P(007)	N(017)	C(026)	72.4(3)
C(00S)	C(02J)	C(03E)	C(02Z)	-0.7(6)	C(03H)	P(007)	C(01B)	C(01K)	158.1(3)
C(00S)	C(02M)	C(049)	C(02Z)	-0.9(6)	C(03H)	P(007)	C(01B)	C(046)	-28.0(3)
C(00T)	P(008)	N(00J)	P(00B)	120.78(16)	C(03H)	C(03T)	C(043)	C(01L)	-1.6(6)
C(00T)	P(008)	N(00J)	C(01X)	-48.8(3)	C(03I)	C(02T)	C(039)	C(03N)	0.6(7)
C(00T)	P(008)	C(01I)	C(029)	163.2(2)	C(03M)	C(033)	C(03A)	C(03C)	0.3(5)
C(00T)	P(008)	C(01I)	C(02X)	-31.3(3)	C(03M)	C(03O)	C(03R)	C(03C)	0.7(6)
C(00T)	C(021)	C(036)	C(04E)	0.8(6)	C(03N)	C(00W)	C(03G)	C(03I)	1.4(5)
C(00T)	C(02E)	C(03L)	C(04E)	0.5(6)	C(03P)	C(024)	C(02R)	C(01Y)	-1.9(5)
C(00W)	P(004)	N(00M)	P(003)	-129.06(15)	C(03S)	C(026)	C(02L)	C(04H)	-1.3(9)
C(00W)	P(004)	N(00M)	C(01Q)	59.0(3)	C(03V)	C(042)	C(10)	C(02U)	-2.2(10)
C(00W)	P(004)	C(01E)	C(02I)	167.6(3)	C(03W)	C(01Z)	C(023)	C(00L)	0.2(6)
C(00W)	P(004)	C(01E)	C(03D)	-16.2(4)	C(03W)	C(03Q)	C(03Z)	C(00L)	2.7(7)
C(00W)	C(03G)	C(03I)	C(02T)	-0.3(6)	C(03Z)	C(00L)	C(023)	C(01Z)	1.5(6)
C(00X)	C(00P)	C(4)	C(9)	0.1(5)	C(03Z)	C(03Q)	C(03W)	C(01Z)	-0.9(8)
C(00X)	C(02A)	C(038)	C(9)	-0.1(6)	C(046)	C(01B)	C(01K)	C(02Y)	-1.3(5)
C(00Y)	C(00R)	C(01C)	S(00C)	-175.2(2)	C(047)	C(041)	C(04H)	C(02L)	1.0(9)
C(00Y)	C(00R)	C(01C)	C(022)	3.4(5)	C(049)	C(02Z)	C(03E)	C(02J)	-1.5(6)
C(00Y)	C(01Q)	C(01T)	C(022)	3.7(5)	C(04C)	S(00C)	C(01C)	C(00R)	-12.3(3)
C(00Z)	P(005)	C(00L)	C(023)	-18.6(3)	C(04C)	S(00C)	C(01C)	C(022)	169.1(3)
C(00Z)	P(005)	C(00L)	C(03Z)	165.5(3)	C(04F)	C(01W)	C(03F)	C(029)	0.4(5)
C(00Z)	P(005)	N(018)	P(009)	-126.33(15)	C(04H)	C(041)	C(047)	C(03S)	-2.3(8)
C(00Z)	P(005)	N(018)	C(00N)	64.5(3)	C(8)	C(014)	C(02Q)	C(02B)	-0.1(5)
C(010)	C(00O)	C(02U)	C(10)	1.1(8)	C(4)	C(00P)	C(00X)	C(02A)	0.2(5)
C(010)	C(03V)	C(042)	C(10)	3.2(9)	C(1)	C(00Z)	C(02C)	C(011)	-1.0(5)
C(011)	C(02P)	C(044)	C(1)	-0.5(6)	C(3)	O(020)	C(02S)	C(1AA)	178.0(4)
C(014)	P(009)	N(018)	P(005)	-116.14(16)	S(4AA)	C(1BA)	C(0BA)	C(5)	-178.6(11)
C(014)	P(009)	N(018)	C(00N)	53.5(3)	C(2)	S(00F)	C(041)	C(047)	8.3(5)
C(014)	P(009)	C(019)	C(016)	-171.5(2)	C(2)	S(00F)	C(041)	C(04H)	-170.7(5)
C(014)	P(009)	C(019)	C(01N)	15.8(3)	C(2BA)	C(1BA)	C(0BA)	C(5)	5(2)
C(014)	C(8)	C(0AA)	C(034)	-0.2(8)	C(1BA)	C(2BA)	C(3BA)	C(026)	10(3)
C(016)	C(019)	C(01N)	C(01A)	1.1(5)	C(1BA)	C(0BA)	C(5)	C(026)	-4.3(19)
N(017)	P(006)	C(00S)	C(02J)	56.4(3)	C(5)	C(026)	C(3BA)	C(2BA)	-11(2)
N(017)	P(006)	C(00S)	C(02M)	-130.3(3)	C(3BA)	C(026)	C(5)	C(0BA)	7.8(19)
N(017)	P(006)	C(01Y)	C(02N)	57.9(3)	C(3BA)	C(2BA)	C(1BA)	S(4AA)	176.8(13)
N(017)	P(006)	C(01Y)	C(02R)	-123.2(2)	C(3BA)	C(2BA)	C(1BA)	C(0BA)	-7(3)
N(017)	P(007)	C(01B)	C(01K)	-89.2(3)	C(4AA)	S(4AA)	C(1BA)	C(2BA)	8.7(18)
N(017)	P(007)	C(01B)	C(046)	84.7(3)	C(4AA)	S(4AA)	C(1BA)	C(0BA)	-167.8(13)

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for first_25.

Atom	*x*	*y*	*z*	U(eq)
H(00R)	6899.8	6056.35	1372.54	30
H(00X)	5852.59	5015.18	3030.81	34
H(00Y)	6857.98	4958.45	1468.32	30
H(010)	4345.58	2365.83	955.97	59
H(011)	661.22	2376.33	3900.26	55
H(016)	3408.41	2944.98	5557.69	32
H(01A)	5280.27	3470.54	6919.21	44
H(01D)	366.59	1655.62	9132.85	48
H(01F)	9136.46	3589.38	1093.05	43
H(01H)	75.67	5621.47	6293.9	34
H(01J)	6096.87	3210.22	5949.26	41
H(01K)	-1129.05	1305.52	6576.28	39
H(01L)	2100.54	1447.07	9109.82	53
H(01M)	7464.49	4223.83	2996.77	33
H(01N)	3536.86	3458.77	7214.6	33
H(01O)	4428.38	834.15	1304.95	35
H(01P)	3059.78	5273.33	5577.1	31

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for first_25.

Atom	*x*	*y*	*z*	U(eq)
H(01R)	-26.89	4543.14	6428.09	31
H(01S)	-265.84	1512.26	8277.83	41
H(01T)	3917.27	5244.39	2300.52	28
H(01W)	5084.23	1781.72	4813.2	44
H(01Z)	-2194.12	4660.04	5490.16	58
H(021)	2945.29	2707.93	1971.8	43
H(022)	3950.54	6337.74	2170.99	30
H(023)	-633.55	4052.93	5189.66	44
H(024)	5473.33	1516.92	5907.16	43
H(025)	7394.76	3600.83	1363.38	35
H(027)	5145.52	2955.36	5267.79	36
H(029)	6086.52	1612.61	3048.47	32
H(02A)	5135.63	5347.01	3994.56	45
H(02B)	1304.32	4713.59	8165.84	47
H(02C)	257.51	2409.86	4932.69	44
H(02D)	9220.66	4189.36	2726.32	44
H(02E)	2866.99	1145.99	3038.55	42
H(02F)	693.95	5099.61	2399.49	58
H(02G)	2934.63	4189.88	5651.33	28
H(02H)	4651.92	-2067.94	2722.79	85
H(02I)	4316.26	-1385.63	3018.31	85
H(02K)	5482.4	-1599.75	2740.71	85
H(02O)	3093.2	3838.72	2603.26	47
H(02J)	242.53	1051.87	5620.76	40
H(02S)	10060.29	3880.45	1775.99	44
H(02L)	977.6	-107.26	5866.36	40
H(02M)	3175.76	618.34	4835.42	41
H(02N)	3433.72	-97.13	5860.25	36
H(02T)	5490.22	565.19	2825.4	33
H(02P)	1678.71	3089.16	3363.33	49
H(02Q)	1942.55	4355.88	7199.33	33
H(02R)	3724.73	1758.78	6030.53	34
H(02)	-1115.14	-254.19	10031.05	78
H	-2253.67	88.56	10111.24	78
H(02U)	5690.17	4130.12	-852.63	67
H(02V)	6741.16	1066.34	453.33	79
H(02W)	1477	4357.59	2978.4	63
H(02X)	3090.23	2041.39	3711.11	36
H(02Y)	-2526.73	749.66	6688.49	52
H(02Z)	967.54	423.6	3937.25	48
H(030)	4259.06	-236.18	1290.94	40
H(031)	1555.01	5345.46	1450.85	69
H(034)	505.12	4041.2	8879	63
H(036)	1258	2674.04	1923.24	67
H(03A)	3092.45	6309.74	5211.18	62
H(03B)	3283.24	6282.68	5875.65	62
H(03C)	2947.64	6947.94	5581.94	62
H(038)	4281	4658.53	4669.98	54
H(039)	4152.68	3771.72	-413.59	66
H(03D)	6894.59	492.29	1510.96	42
H(03F)	5284.19	-508.21	2820.99	37
H(03G)	8566.45	30.53	1348.05	46
H(03H)	3169.49	4846.79	1081.42	55
H(03E)	-262.16	786.85	4764.2	50
H(03I)	6405.18	1576.45	4005	43
H(03J)	6278.23	4380.88	769.35	38
H(03K)	6754.32	4425.5	-260.38	54
H(03L)	1163	1133.76	2997.38	63
H(03M)	7866.67	2226.14	1292.91	42
H(03N)	3667.72	3721.78	616.49	48
H(03O)	9531.04	1756.89	1096.66	54

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for first_25.

Atom	*x*	*y*	*z*	U(eq)
H(03P)	6193.29	473.5	5781.91	45
H(03Q)	-2474.39	3851.67	7112.28	73
H(03R)	9888.37	657.32	1133.13	48
H(03S)	1972.57	-92.48	7401.69	38
H(03T)	2590.49	994.32	7382.57	43
H(03V)	3860.02	2275.22	60.19	75
H(03W)	-3111.15	4564.68	6448.76	66
H(03Z)	-958.76	3212.82	6810.87	55
H(040)	-2784.23	-17.56	7428.12	59
H(042)	4869.51	1630.57	-669.23	80
H(043)	3196.74	1112.05	8246.96	55
H(044)	2266.25	3850.31	3858.33	59
H(046)	-213.62	299.97	7935.81	43
H(047)	2005.13	-1185.53	7470.79	38
H(049)	2668.55	374.69	3966.56	50
H(04B)	5179.35	-338.15	5769.3	46
H(04A)	6900.9	7096.52	1014.99	80
H(04C)	7020.41	7101.71	1692.1	80
H(04E)	6649.51	7744.95	1375.46	80
H(04D)	-1669.26	-217.87	8081.07	60
H(04F)	372.04	1891.82	2442.99	73
H(04G)	3428.72	2008.74	4666.65	46
H(04H)	1074.58	-1194.71	5923.67	43
H(8)	935.27	2661.33	7679	52
H(10)	6273.12	1000.91	-463.09	106
H(4)	4856.63	3296.83	3427.81	41
H(9)	4131.81	3638.87	4389.61	56
H(1)	1825.51	3914.3	4890.36	53
H(0AA)	306.29	3024.93	8639.28	78
H(1AA)	-1682.95	851.47	9377.38	113
H(1AB)	-547.44	520.12	9332.89	113
H(1AC)	-1139.19	862.88	9931.53	113
H(3A)	-2775.23	-877.3	9769.67	87
H(3B)	-1627.43	-1186.06	9736.77	87
H(3AA)	-1463.46	-1352.17	8727.69	116
H(3AB)	-2610.8	-1047.26	8762.75	116
H(3AC)	-2371.17	-1702.23	9100.66	116
H(2A)	2511.5	-2310.4	7432.38	62
H(2B)	1756.02	-2837.11	7458.96	62
H(2C)	1332.27	-2142.39	7707.18	62
H(2BA)	893.19	-1238.69	6282.51	38
H(0BA)	2499.57	-1017.26	7538.94	25
H(5)	2317.86	113.19	7344.31	14
H(3BA)	629.46	-115.82	6159.12	35
H(4AA)	1739.23	-2276.17	6213.13	106
H(4AB)	628.1	-2227.94	6618.85	106
H(4AC)	1414.4	-2846.31	6655.96	106

Table 8 Atomic Occupancy for first_25.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
S(00F)	0.746(4)	C(02L)	0.746(4)	H(02L)	0.746(4)
C(03S)	0.746(4)	H(03S)	0.746(4)	C(041)	0.746(4)
C(047)	0.746(4)	H(047)	0.746(4)	C(04H)	0.746(4)
H(04H)	0.746(4)	S(4AA)	0.254(4)	C(2)	0.719(12)
H(2A)	0.719(12)	H(2B)	0.719(12)	H(2C)	0.719(12)
C(2BA)	0.254(4)	H(2BA)	0.254(4)	C(1BA)	0.254(4)
C(0BA)	0.254(4)	H(0BA)	0.254(4)	C(5)	0.254(4)
H(5)	0.254(4)	C(3BA)	0.254(4)	H(3BA)	0.254(4)
C(4AA)	0.259(14)	H(4AA)	0.259(14)	H(4AB)	0.259(14)
H(4AC)	0.259(14)				

Table 9 Solvent masks information for first_25.

Number	X	Y	Z	Volume	Electron count	Content
1	0.000	0.500	0.000	632.4	65.1	?
2	0.500	0.000	1.000	70.5	10.5	?

5.3 Details and Tables for 3

Single crystals of $C_{124}H_{108}Au_2F_{12}N_4P_{10}S_4$ [marco1] were submitted for single crystal X-ray determination. A suitable crystal was selected and mounted on a MiTeGen tip via Parabol oil and placed on a XtaLAB AFC12 (RCD3): Kappa single diffractometer. The crystal was kept at 109(14) K during data collection. Using Olex2,[4] the structure was solved with the XT[5] structure solution program using Intrinsic Phasing and refined with the XL[6] refinement package using Least Squares minimisation. For the measurement, the crystals presented as very fine needles and crystal screening demonstrated that the sample contained twinned multiples. Thus, the model was refined against an HKLF 5 reflection set.

Crystal Data for $C_{124}H_{108}Au_2F_{12}N_4P_{10}S_4$ (*M* =2714.01 g/mol): triclinic, space group P-1 (no. 2), *a* = 12.2295(3) Å, *b* = 21.7084(6) Å, *c* = 24.2101(5) Å, *α* = 74.296(2)°, *β* = 89.995(2)°, *γ* = 74.781(2)°, *V* = 5953.0(3) Å^3, *Z* = 2, *T* = 109(14) K, μ(Mo Kα) = 2.735 mm^{-1}, *Dcalc* = 1.514 g/cm^3, 24260 reflections measured (3.462° ≤ 2Θ ≤ 52.742°), 24260 unique (R_{int} = ?, R_{sigma} = 0.0496) which were used in all calculations. The final R_1 was 0.0971 (I > 2σ(I)) and wR_2 was 0.2983 (all data).

Table 1 Crystal data and structure refinement for marco1.

Identification code	marco1
Empirical formula	$C_{124}H_{108}Au_2F_{12}N_4P_{10}S_4$
Formula weight	2714.01
Temperature/K	109(14)
Crystal system	triclinic
Space group	P-1
a/Å	12.2295(3)
b/Å	21.7084(6)
c/Å	24.2101(5)
α/°	74.296(2)
β/°	89.995(2)
γ/°	74.781(2)
Volume/Å^3	5953.0(3)
Z	2
ρ_{calc}g/cm^3	1.514
μ/mm^{-1}	2.735
F(000)	2720.0
Crystal size/mm^3	0.1 × 0.01 × 0.005
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	3.462 to 52.742
Index ranges	-15 ≤ h ≤ 15, -25 ≤ k ≤ 26, 0 ≤ l ≤ 30
Reflections collected	24260
Independent reflections	24260 [R_{int} = ?, R_{sigma} = 0.0496]
Data/restraints/parameters	24260/270/1410

Goodness-of-fit on F^2	1.355
Final R indexes [I>=2σ (I)]	R_1 = 0.0971, wR_2 = 0.2869
Final R indexes [all data]	R_1 = 0.1033, wR_2 = 0.2983
Largest diff. peak/hole / e Å^{-3}	7.50/-3.41

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for marco1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Au(1)	3689.1(3)	7513.4(2)	5625.2(2)	11.86(14)
Au(2)	3776.6(3)	7485.0(2)	732.1(2)	12.97(14)
P(100)	8850(2)	7460.9(13)	3153.5(11)	13.9(5)
P(101)	8761(2)	7547.0(13)	8164.2(11)	15.6(6)
P(3)	5307(2)	6550.8(12)	5841.0(11)	9.9(5)
P(7)	3414(2)	8493.6(12)	1026.2(11)	11.8(5)
P(2)	3161(2)	8486.9(12)	4814.7(11)	10.9(5)
P(8)	3251(2)	8446.6(12)	-97.9(11)	9.9(5)
P(4)	3084(2)	6515.2(12)	5934.9(11)	9.9(5)
P(5)	3138(2)	6494.0(12)	987.2(11)	10.8(5)
P(6)	5381(2)	6506.6(12)	903.0(11)	11.2(5)
P(1)	3297(2)	8505.5(12)	5946.3(11)	9.8(5)
S(1)	2223(2)	11967.2(12)	4398.3(14)	27.6(6)
S(4)	780(2)	11908.0(12)	-486.8(13)	27.5(6)
S(3)	5760(3)	3042.5(14)	1374.1(13)	26.0(7)
S(2)	5897(3)	3060.1(14)	6412.6(14)	26.7(7)
F(1)	7547(5)	7425(3)	3107(2)	15.6(13)
F(10)	8688(5)	7538(4)	8818(3)	21.5(14)
F(12)	7435(5)	7540(3)	8118(3)	19.6(13)
F(6)	8921(6)	7476(4)	2484(3)	30.4(16)
F(9)	10056(5)	7549(4)	8185(3)	21.3(14)
F(7)	8804(5)	7556(4)	7490(3)	25.2(15)
F(5)	8407(6)	8265(3)	2960(4)	31.7(18)
F(8)	8368(6)	8355(3)	7955(3)	25.5(15)
F(11)	9143(6)	6743(3)	8346(3)	23.9(15)
F(2)	9291(6)	6666(3)	3327(3)	23.8(15)
F(3)	8765(6)	7444(4)	3809(3)	23.6(14)
F(4)	10130(5)	7489(4)	3183(3)	22.5(14)
N(1)	3061(7)	9009(4)	5240(4)	11.6(17)
N(3)	4493(7)	5997(4)	1033(4)	11.5(17)
N(4)	3048(8)	8980(4)	331(4)	14.8(18)
C(100)	4841(9)	5286(5)	1127(4)	15(2)
N(2)	4449(7)	6024(4)	6003(4)	11.2(17)
C(125)	2265(9)	6337(5)	460(5)	17(2)
C(26)	5316(9)	8236(6)	6556(5)	17(2)
C(42)	6859(10)	6680(6)	4360(5)	24(3)
C(33)	4833(9)	5311(5)	6115(4)	12.6(18)
C(53)	1860(9)	6821(5)	6809(5)	18(2)
C(47)	5772(10)	6355(6)	7008(5)	21(2)
C(49)	7524(10)	6422(5)	7410(6)	28(3)
C(120)	1904(9)	6685(5)	1894(5)	19(2)
C(139)	1376(9)	8191(6)	-532(5)	22(2)
C(144)	4331(9)	8616(5)	-575(5)	16(2)
C(134)	2619(9)	10773(5)	-418(5)	25(2)
C(138)	1981(9)	8667(5)	-561(4)	15(2)
C(111)	6969(10)	6672(6)	-569(5)	22(2)
C(27)	1992(9)	8707(5)	6303(5)	17(2)
C(1)	2829(9)	9709(5)	5063(4)	14.3(17)
C(132)	2549(8)	9681(5)	127(4)	15(2)
C(25)	6159(9)	8361(6)	6862(5)	20(2)
C(142)	618(10)	9420(6)	-1343(5)	31(3)
C(9)	1279(9)	9389(5)	4080(5)	20(2)
C(17)	5859(10)	8657(5)	3516(6)	25.1(19)

Table 2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for marco1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C(62)	1709(12)	6368(7)	4463(6)	32(2)
C(126)	2570(10)	6439(5)	-107(5)	17(2)
C(28)	975(9)	8698(5)	6049(5)	25(3)
C(46)	6261(8)	6393(5)	6475(4)	14(2)
C(13)	1332(9)	8217(6)	4365(5)	22(2)
C(135)	1513(8)	11059(4)	-292(4)	17(2)
C(121)	1335(10)	6518(6)	2387(5)	28(3)
C(21)	4342(9)	8731(5)	6313(4)	15(2)
C(6)	3615(9)	10010(5)	4766(5)	17.7(19)
C(143)	1595(9)	9292(5)	-985(5)	20(2)
C(123)	2025(10)	5357(6)	2407(5)	26(3)
C(19)	3400(8)	10690(4)	4570(5)	19(2)
C(136)	934(8)	10630(4)	54(4)	17(2)
C(153)	5400(10)	9556(6)	1506(5)	32(3)
C(145)	5330(8)	8703(5)	-344(5)	16(2)
C(161)	2245(9)	8709(5)	1470(5)	16(2)
C(63)	2458(11)	6419(6)	4861(5)	23(2)
C(140)	421(9)	8330(6)	-896(6)	24(3)
C(4)	2393(9)	11112(4)	4689(5)	18.7(19)
C(112)	6283(9)	6785(5)	-142(5)	19(2)
C(133)	3132(9)	10103(5)	-207(5)	19(2)
C(14)	4173(9)	8641(5)	4280(5)	17.5(17)
C(51)	7374(9)	6442(5)	6407(5)	22(2)
C(113)	6336(9)	6283(5)	1542(5)	15.3(17)
C(108)	7024(9)	5653(5)	422(5)	19(2)
C(20)	5292(8)	8579(5)	4481(5)	16.6(17)
C(54)	1293(9)	6715(5)	7313(5)	21(2)
C(45)	6997(8)	5701(5)	5388(5)	19(2)
C(116)	7659(11)	6196(6)	2514(5)	30(2)
C(127)	1856(11)	6419(6)	-534(6)	30(3)
C(115)	6510(11)	6225(6)	2558(5)	24(2)
C(150)	5427(9)	8241(6)	1638(5)	21(2)
C(44)	7679(10)	5562(6)	4948(6)	27(3)
C(12)	336(10)	8368(6)	4024(5)	23(2)
C(154)	4533(10)	9411(5)	1244(5)	22(2)
C(24)	6019(10)	8999(6)	6921(6)	30(3)
C(8)	1805(9)	8730(5)	4395(4)	15.2(18)
C(41)	6170(9)	6803(5)	4788(5)	18(2)
C(55)	1345(10)	6064(6)	7622(6)	27(3)
C(107)	6303(9)	6277(5)	359(5)	15(2)
C(30)	53(11)	8729(6)	6907(6)	38(4)
C(61)	737(11)	6181(6)	4627(6)	31(2)
C(160)	1263(10)	8518(5)	1382(5)	26(3)
C(151)	6308(10)	8388(7)	1910(5)	30(3)
C(146)	6234(9)	8730(5)	-685(5)	26(3)
C(118)	7486(9)	6249(5)	1506(5)	22(2)
C(114)	5856(10)	6269(6)	2083(5)	20(2)
C(131)	1443(8)	9961(4)	248(4)	17(2)
C(18)	6136(10)	8598(6)	4086(5)	26(2)
C(158)	496(11)	8828(6)	2208(6)	30(3)
C(3)	1613(9)	10812(5)	5005(5)	22(2)
C(119)	2532(9)	6192(6)	1659(5)	17(2)
C(124)	2580(9)	5534(6)	1920(5)	24(2)
C(40)	6226(9)	6309(5)	5301(5)	13(2)
C(147)	6195(12)	8668(6)	-1239(7)	39(4)
C(43)	7619(10)	6064(6)	4441(6)	27(3)
C(57)	2553(9)	5653(6)	6945(5)	20(2)
C(104)	4858(9)	4327(5)	803(5)	16(2)
C(34)	4578(9)	5010(5)	5712(5)	17.8(19)
C(23)	5050(9)	9503(6)	6668(5)	25(2)

Table 2 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for marco1. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C(10)	267(9)	9518(6)	3747(5)	27(2)
C(52)	2490(9)	6300(5)	6616(5)	14(2)
C(159)	390(11)	8578(5)	1742(6)	35(3)
C(2)	1817(9)	10125(5)	5184(4)	19(2)
C(155)	4559(9)	8734(5)	1319(4)	17(2)
C(58)	2233(9)	6282(5)	5450(5)	17.6(18)
C(32)	2028(9)	8747(5)	6875(5)	26(3)
C(152)	6283(11)	9039(7)	1844(6)	32(3)
C(137)	1733(12)	12274(6)	-918(8)	62(5)
C(38)	5458(9)	4915(5)	6620(5)	18(2)
C(141)	59(10)	8935(6)	-1299(6)	31(3)
C(117)	8144(11)	6213(6)	1998(5)	32(3)
C(128)	785(11)	6320(6)	-412(6)	34(3)
C(29)	38(10)	8706(5)	6356(6)	31(3)
C(101)	5461(9)	4862(5)	1628(5)	16(2)
C(102)	5795(10)	4178(5)	1722(5)	20(2)
C(148)	5214(10)	8583(5)	-1462(5)	27(3)
C(22)	4207(9)	9372(5)	6370(5)	23(2)
C(122)	1371(10)	5854(6)	2635(5)	29(3)
C(56)	2004(10)	5534(6)	7444(5)	25(3)
C(109)	7705(10)	5528(6)	-15(6)	25(3)
C(105)	4566(9)	5006(5)	710(5)	17(2)
C(37)	5837(9)	4222(5)	6729(5)	18(2)
C(130)	1192(10)	6239(6)	580(5)	25(2)
C(35)	4917(9)	4328(5)	5810(5)	18.3(19)
C(59)	1236(10)	6099(6)	5607(6)	27(2)
C(129)	478(11)	6213(6)	153(6)	36(3)
C(110)	7693(10)	6046(6)	-510(5)	23(3)
C(50)	7978(10)	6450(6)	6894(6)	31(3)
C(149)	4287(10)	8561(5)	-1130(5)	24(2)
C(15)	3924(9)	8716(5)	3707(5)	21.3(19)
C(31)	1080(10)	8744(6)	7184(5)	31(3)
C(48)	6415(10)	6363(6)	7475(5)	25(2)
C(16)	4770(10)	8716(6)	3321(6)	32(2)
C(103)	5466(9)	3899(5)	1300(5)	17(2)
C(11)	-196(10)	9006(6)	3716(5)	27(2)
C(60)	510(10)	6029(5)	5208(6)	26(2)
C(156)	2326(9)	8979(5)	1924(5)	23(2)
C(36)	5542(9)	3928(6)	6323(5)	18.6(19)
C(39)	6825(13)	2706(7)	7063(6)	38(3)
C(157)	1461(10)	9031(6)	2293(5)	33(3)
C(7)	966(12)	12316(6)	4710(7)	58(5)
C(106)	6759(13)	2656(8)	2002(7)	46(4)

Table 3 Anisotropic Displacement Parameters (Å²×10³) for marco1. 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}
Au(1)	17.6(2)	1.4(2)	14.3(2)	-0.28(16)	-0.13(14)	-0.76(15)
Au(2)	17.2(2)	2.3(2)	17.3(2)	-1.04(15)	-0.48(15)	-0.83(16)
P(100)	18.0(13)	15.7(14)	9.3(12)	-4.7(11)	-1.8(10)	-5.7(11)
P(101)	17.8(13)	20.5(15)	11.9(13)	-6.5(12)	4.4(10)	-8.8(12)
P(3)	13.3(12)	4.5(11)	9.3(12)	0.0(9)	-2.2(9)	0.2(9)
P(7)	15.1(12)	4.6(11)	14.1(13)	-1.2(9)	1.6(10)	-1.8(9)
P(2)	16.9(12)	3.0(11)	12.0(12)	-0.9(9)	0.7(9)	-2.9(9)
P(8)	15.4(12)	1.4(11)	11.3(12)	0.2(9)	-0.3(9)	-1.5(9)
P(4)	12.8(12)	2.4(11)	12.6(12)	-0.8(9)	0.4(9)	-0.3(9)
P(5)	12.8(12)	2.7(11)	16.3(13)	-3.4(9)	0.6(10)	-0.1(9)
P(6)	14.4(12)	4.4(11)	12.9(12)	-0.1(9)	-0.4(9)	-1.6(9)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for marco1. 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}
$P^{(1)}$	13.8(12)	3.4(11)	11.9(12)	-2.0(9)	0.2(9)	-2.2(9)
$S^{(1)}$	33.2(15)	8.1(11)	37.3(17)	-0.4(11)	8.9(13)	-4.5(10)
$S^{(4)}$	30.0(15)	9.0(12)	36.3(17)	1.1(11)	0.4(12)	-0.8(10)
$S^{(3)}$	40.8(17)	7.6(13)	25.4(15)	-2.2(11)	-5.7(13)	-1.9(11)
$S^{(2)}$	40.6(17)	7.4(13)	28.2(16)	-3.0(11)	-0.9(13)	-1.9(11)
$F^{(1)}$	18(3)	25(3)	2(2)	0(2)	-3(2)	-8(2)
$F^{(10)}$	22(3)	27(4)	19(3)	-6(3)	0(2)	-13(3)
$F^{(12)}$	15(3)	23(3)	16(3)	3(3)	9(2)	-4(2)
$F^{(6)}$	24(3)	50(5)	19(4)	-14(3)	1(3)	-8(3)
$F^{(9)}$	13(3)	39(4)	19(3)	-16(3)	2(2)	-11(3)
$F^{(7)}$	18(3)	46(4)	16(3)	-13(3)	6(2)	-12(3)
$F^{(5)}$	26(4)	19(4)	54(5)	-13(3)	19(3)	-9(3)
$F^{(8)}$	29(4)	16(3)	33(4)	-8(3)	13(3)	-9(3)
$F^{(11)}$	33(4)	12(3)	26(4)	-6(3)	-7(3)	-4(3)
$F^{(2)}$	33(4)	15(3)	23(4)	-6(3)	-9(3)	-6(3)
$F^{(3)}$	28(3)	28(4)	22(4)	-13(3)	5(3)	-14(3)
$F^{(4)}$	15(3)	26(4)	35(4)	-20(3)	11(3)	-8(3)
$N^{(1)}$	13(4)	2(4)	18(4)	-2(3)	-4(3)	2(3)
$N^{(3)}$	10(4)	13(4)	12(4)	-3(3)	1(3)	-4(3)
$N^{(4)}$	21(4)	6(4)	16(4)	-1(3)	1(3)	-2(3)
$C^{(100)}$	17(5)	12(5)	9(5)	3(4)	-2(4)	-1(4)
$N^{(2)}$	12(4)	5(4)	14(4)	0(3)	-2(3)	0(3)
$C^{(125)}$	13(5)	17(5)	18(5)	-8(4)	-7(4)	5(4)
$C^{(26)}$	18(2)	17(2)	17(2)	-4.7(11)	0.9(10)	-4.6(11)
$C^{(42)}$	26(6)	14(6)	26(6)	2(5)	4(5)	-5(5)
$C^{(33)}$	17(4)	6(3)	12(3)	0(2)	-1(3)	0(3)
$C^{(53)}$	19(5)	16(5)	14(5)	-2(4)	1(4)	1(4)
$C^{(47)}$	21(5)	18(5)	17(6)	-4(4)	-5(4)	4(4)
$C^{(49)}$	29(6)	19(6)	34(7)	-7(5)	-12(5)	-6(5)
$C^{(120)}$	21(5)	13(5)	21(6)	-8(4)	-1(4)	2(4)
$C^{(139)}$	21(5)	13(5)	33(7)	-10(5)	10(5)	-4(4)
$C^{(144)}$	20(5)	6(4)	22(6)	-2(4)	7(4)	-7(4)
$C^{(134)}$	30(6)	23(5)	22(6)	-4(5)	5(5)	-9(5)
$C^{(138)}$	16(5)	15(5)	12(5)	0(4)	-5(4)	-6(4)
$C^{(111)}$	26(6)	11(5)	22(6)	5(4)	-5(5)	-5(4)
$C^{(27)}$	18(5)	7(4)	22(5)	2(4)	10(4)	-5(3)
$C^{(1)}$	20(3)	8(3)	14(4)	-2(3)	-1(3)	-4(2)
$C^{(132)}$	21(5)	7(4)	13(5)	0(4)	-1(4)	-3(4)
$C^{(25)}$	19(5)	22(6)	13(5)	4(4)	-10(4)	-3(4)
$C^{(142)}$	33(7)	28(6)	20(6)	-3(5)	-14(5)	6(5)
$C^{(9)}$	22(4)	19(3)	16(4)	1(3)	-5(3)	-4(3)
$C^{(17)}$	32(3)	7(5)	33(4)	-6(4)	12(3)	-2(3)
$C^{(62)}$	39(5)	25(6)	29(4)	-9(4)	-11(3)	-5(4)
$C^{(126)}$	22(5)	11(5)	14(5)	-4(4)	-6(4)	-1(4)
$C^{(28)}$	22(6)	13(5)	37(7)	-7(5)	6(5)	-2(4)
$C^{(46)}$	18(5)	8(4)	13(5)	-4(4)	-3(4)	-1(4)
$C^{(13)}$	19(4)	21(3)	31(5)	-11(3)	-3(3)	-8(3)
$C^{(135)}$	14(5)	13(5)	22(6)	-5(4)	-7(4)	-1(4)
$C^{(121)}$	15(5)	40(8)	22(6)	-6(5)	1(4)	1(5)
$C^{(21)}$	16(5)	21(5)	6(5)	3(4)	2(4)	-9(4)
$C^{(6)}$	23(4)	6(3)	24(5)	-5(3)	5(3)	-3(2)
$C^{(143)}$	29(6)	13(5)	17(5)	2(4)	-3(4)	-7(4)
$C^{(123)}$	30(6)	21(6)	24(6)	3(5)	7(5)	-11(5)
$C^{(19)}$	22(4)	6(3)	28(5)	-4(3)	3(3)	-3(2)
$C^{(136)}$	14(5)	13(5)	25(6)	-8(4)	0(4)	0(4)
$C^{(153)}$	43(7)	29(6)	24(7)	-4(5)	-2(5)	-15(5)
$C^{(145)}$	13(5)	13(5)	23(6)	-5(4)	3(4)	-4(4)
$C^{(161)}$	26(5)	6(4)	15(5)	-2(4)	5(4)	-4(4)
$C^{(63)}$	31(4)	13(5)	26(4)	-10(3)	-4(3)	-1(4)
$C^{(140)}$	15(5)	24(6)	40(7)	-19(5)	1(5)	-6(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for marco1. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
$C^{(4)}$	24(4)	6(3)	25(5)	-5(3)	2(3)	-2(2)
$C^{(112)}$	23(6)	8(5)	22(6)	2(4)	-3(4)	-6(4)
$C^{(133)}$	27(6)	8(5)	25(6)	-3(4)	4(4)	-10(4)
$C^{(14)}$	17.6(19)	17(2)	17.9(19)	-5.2(11)	1.7(10)	-4.0(10)
$C^{(51)}$	16(5)	20(5)	25(6)	6(4)	-5(4)	-7(4)
$C^{(113)}$	16.0(18)	14.9(19)	15.5(18)	-4.1(10)	0.7(10)	-5.1(10)
$C^{(108)}$	12(5)	15(5)	27(6)	-4(4)	-1(4)	-2(4)
$C^{(20)}$	14(2)	6(4)	25(3)	-1(3)	1.4(19)	2(2)
$C^{(54)}$	22(5)	12(5)	30(6)	-10(4)	8(5)	-5(4)
$C^{(45)}$	9(5)	15(5)	28(6)	-1(4)	-3(4)	-1(4)
$C^{(116)}$	38(4)	30(6)	22(4)	-2(4)	-9(3)	-15(4)
$C^{(127)}$	40(7)	21(6)	26(7)	-6(5)	-12(5)	0(5)
$C^{(115)}$	37(4)	20(5)	19(3)	-7(4)	-4(3)	-11(3)
$C^{(150)}$	16(5)	24(6)	26(6)	-6(5)	-2(4)	-11(4)
$C^{(44)}$	25(6)	17(6)	37(7)	-8(5)	7(5)	1(5)
$C^{(12)}$	19(4)	29(4)	28(5)	-16(3)	-1(3)	-10(3)
$C^{(154)}$	35(6)	11(5)	24(6)	-6(4)	-1(5)	-11(4)
$C^{(24)}$	31(6)	31(7)	33(7)	-11(5)	1(5)	-16(5)
$C^{(8)}$	17(4)	17(3)	12(4)	-1(3)	-3(3)	-7(2)
$C^{(41)}$	21(5)	10(5)	24(6)	-4(4)	4(4)	-5(4)
$C^{(55)}$	29(6)	23(6)	27(7)	-3(5)	8(5)	-6(5)
$C^{(107)}$	20(5)	12(5)	14(5)	-5(4)	0(4)	-4(4)
$C^{(30)}$	32(7)	20(6)	49(9)	10(6)	20(6)	-4(5)
$C^{(61)}$	37(5)	19(5)	38(4)	-13(4)	-11(3)	-3(4)
$C^{(160)}$	35(6)	23(6)	26(6)	-9(5)	9(5)	-13(5)
$C^{(151)}$	23(6)	41(8)	13(6)	5(5)	-12(5)	2(5)
$C^{(146)}$	19(5)	22(6)	40(7)	-13(5)	5(5)	-4(4)
$C^{(118)}$	18(2)	27(6)	19(4)	0(4)	-4(2)	-11(3)
$C^{(114)}$	25(3)	22(5)	15(2)	-6(3)	1(2)	-8(4)
$C^{(131)}$	23(5)	10(4)	16(5)	-1(4)	1(4)	-4(4)
$C^{(18)}$	24(3)	19(5)	35(4)	-8(4)	12(3)	-6(4)
$C^{(158)}$	38(7)	17(6)	32(7)	-1(5)	18(6)	-7(5)
$C^{(3)}$	25(4)	10(3)	28(5)	-2(3)	5(4)	-2(3)
$C^{(119)}$	15(5)	17(5)	23(6)	-14(4)	0(4)	-4(4)
$C^{(124)}$	18(5)	24(6)	29(6)	-7(5)	3(5)	-4(4)
$C^{(40)}$	13(5)	15(5)	17(5)	-10(4)	0(4)	-6(4)
$C^{(147)}$	57(9)	15(6)	50(9)	-12(6)	29(7)	-17(6)
$C^{(43)}$	23(6)	24(7)	38(7)	-18(6)	13(5)	-1(5)
$C^{(57)}$	15(5)	19(5)	28(6)	-8(5)	3(4)	-8(4)
$C^{(104)}$	16(5)	13(5)	16(5)	-5(4)	-2(4)	-1(4)
$C^{(34)}$	23(5)	14(3)	18(4)	-6(3)	1(3)	-5(3)
$C^{(23)}$	26(3)	25(3)	25(3)	-7.1(12)	1.5(10)	-7.4(12)
$C^{(10)}$	24(4)	26(4)	25(5)	-3(3)	-10(4)	-2(3)
$C^{(52)}$	12(5)	15(5)	14(5)	-6(4)	-5(4)	2(4)
$C^{(159)}$	29(7)	14(6)	55(9)	-1(6)	24(6)	-5(5)
$C^{(2)}$	24(4)	11(3)	19(5)	-1(3)	4(3)	-2(2)
$C^{(155)}$	24(6)	17(5)	9(5)	-2(4)	3(4)	-8(4)
$C^{(58)}$	14(3)	9(4)	26(3)	-8(3)	-6(3)	7(3)
$C^{(32)}$	19(5)	21(6)	28(6)	3(5)	3(5)	1(4)
$C^{(152)}$	31(7)	53(8)	30(7)	-23(6)	4(5)	-27(6)
$C^{(137)}$	50(9)	28(7)	100(15)	-5(8)	31(10)	-12(6)
$C^{(38)}$	25(5)	9(3)	15(3)	3(3)	-4(3)	0(3)
$C^{(141)}$	28(6)	32(7)	35(7)	-18(6)	-4(5)	-4(5)
$C^{(117)}$	31(4)	42(7)	23(4)	-2(4)	-8(3)	-19(4)
$C^{(128)}$	35(7)	18(6)	42(8)	-9(5)	-21(6)	1(5)
$C^{(29)}$	26(6)	23(6)	44(8)	-6(5)	7(5)	-10(5)
$C^{(101)}$	23(5)	9(5)	16(5)	0(4)	3(4)	-5(4)
$C^{(102)}$	26(6)	10(5)	16(5)	5(4)	-5(4)	-1(4)
$C^{(148)}$	42(7)	16(5)	24(6)	-7(5)	14(5)	-7(5)
$C^{(22)}$	24(6)	14(5)	26(6)	-5(4)	-2(5)	4(4)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for marco1. 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}
$C^{(122)}$	29(6)	37(7)	24(6)	-12(5)	5(5)	-11(5)
$C^{(56)}$	23(6)	27(6)	21(6)	3(5)	0(4)	-9(5)
$C^{(109)}$	27(6)	17(6)	31(7)	-8(5)	6(5)	-4(5)
$C^{(105)}$	14(5)	15(5)	23(6)	-8(4)	-1(4)	-6(4)
$C^{(37)}$	23(5)	9(3)	17(4)	3(3)	-5(3)	0(3)
$C^{(130)}$	27(6)	26(6)	26(6)	-13(5)	0(5)	-8(5)
$C^{(35)}$	23(5)	14(3)	19(4)	-7(3)	0(3)	-5(3)
$C^{(59)}$	21(4)	28(6)	35(4)	-16(4)	-3(3)	-6(4)
$C^{(129)}$	30(7)	33(7)	53(9)	-26(7)	-8(6)	-5(5)
$C^{(110)}$	27(6)	13(6)	32(7)	-10(5)	12(5)	-8(5)
$C^{(50)}$	30(6)	24(6)	45(8)	-7(6)	-1(5)	-19(5)
$C^{(149)}$	31(6)	23(6)	23(6)	-11(5)	7(5)	-11(5)
$C^{(15)}$	28(3)	18(5)	18(2)	-6(3)	2.0(19)	-4(3)
$C^{(31)}$	41(7)	26(6)	15(6)	1(5)	10(5)	3(5)
$C^{(48)}$	34(6)	19(6)	19(6)	-4(5)	-7(5)	-1(5)
$C^{(16)}$	37(4)	32(6)	26(3)	-11(4)	12(3)	-8(3)
$C^{(103)}$	14(5)	14(5)	25(6)	-5(4)	-1(4)	-6(4)
$C^{(11)}$	20(4)	34(4)	27(5)	-13(3)	0(3)	-5(3)
$C^{(60)}$	23(4)	14(5)	39(4)	-12(3)	-11(3)	2(3)
$C^{(156)}$	26(6)	12(5)	23(6)	-1(4)	-1(4)	4(4)
$C^{(36)}$	18(4)	17(4)	21(4)	-4(3)	2(3)	-4(3)
$C^{(39)}$	52(8)	23(6)	35(8)	-6(5)	-4(6)	-5(5)
$C^{(157)}$	37(7)	36(7)	18(6)	-8(5)	3(5)	3(5)
$C^{(7)}$	50(9)	28(7)	80(13)	-4(7)	34(9)	6(6)
$C^{(106)}$	47(4)	44(4)	45(4)	-12(2)	2(2)	-12(2)

Table 4 Bond Lengths for marco1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
$Au^{(1)}$	$P^{(3)}$	2.407(2)	$C^{(132)}$	$C^{(131)}$	1.397(13)
$Au^{(1)}$	$P^{(2)}$	2.402(2)	$C^{(25)}$	$C^{(24)}$	1.397(17)
$Au^{(1)}$	$P^{(4)}$	2.402(2)	$C^{(142)}$	$C^{(143)}$	1.397(15)
$Au^{(1)}$	$P^{(1)}$	2.416(2)	$C^{(142)}$	$C^{(141)}$	1.379(18)
$Au^{(2)}$	$P^{(7)}$	2.415(2)	$C^{(9)}$	$C^{(8)}$	1.403(15)
$Au^{(2)}$	$P^{(8)}$	2.415(2)	$C^{(9)}$	$C^{(10)}$	1.398(15)
$Au^{(2)}$	$P^{(5)}$	2.405(2)	$C^{(17)}$	$C^{(18)}$	1.384(18)
$Au^{(2)}$	$P^{(6)}$	2.422(2)	$C^{(17)}$	$C^{(16)}$	1.376(17)
$P^{(100)}$	$F^{(1)}$	1.622(6)	$C^{(62)}$	$C^{(63)}$	1.375(17)
$P^{(100)}$	$F^{(6)}$	1.615(7)	$C^{(62)}$	$C^{(61)}$	1.38(2)
$P^{(100)}$	$F^{(5)}$	1.618(7)	$C^{(126)}$	$C^{(127)}$	1.371(16)
$P^{(100)}$	$F^{(2)}$	1.601(7)	$C^{(28)}$	$C^{(29)}$	1.364(15)
$P^{(100)}$	$F^{(3)}$	1.583(7)	$C^{(46)}$	$C^{(51)}$	1.400(14)
$P^{(100)}$	$F^{(4)}$	1.584(7)	$C^{(13)}$	$C^{(12)}$	1.385(16)
$P^{(101)}$	$F^{(10)}$	1.580(7)	$C^{(13)}$	$C^{(8)}$	1.399(15)
$P^{(101)}$	$F^{(12)}$	1.630(7)	$C^{(135)}$	$C^{(136)}$	1.412(13)
$P^{(101)}$	$F^{(9)}$	1.586(6)	$C^{(121)}$	$C^{(122)}$	1.391(17)
$P^{(101)}$	$F^{(7)}$	1.629(7)	$C^{(21)}$	$C^{(22)}$	1.402(15)
$P^{(101)}$	$F^{(8)}$	1.624(7)	$C^{(6)}$	$C^{(19)}$	1.376(12)
$P^{(101)}$	$F^{(11)}$	1.617(7)	$C^{(123)}$	$C^{(124)}$	1.374(16)
$P^{(3)}$	$N^{(2)}$	1.718(9)	$C^{(123)}$	$C^{(122)}$	1.407(16)
$P^{(3)}$	$C^{(46)}$	1.827(10)	$C^{(19)}$	$C^{(4)}$	1.410(12)
$P^{(3)}$	$C^{(40)}$	1.818(11)	$C^{(136)}$	$C^{(131)}$	1.370(12)
$P^{(7)}$	$N^{(4)}$	1.714(9)	$C^{(153)}$	$C^{(154)}$	1.381(16)
$P^{(7)}$	$C^{(161)}$	1.827(10)	$C^{(153)}$	$C^{(152)}$	1.402(18)
$P^{(7)}$	$C^{(155)}$	1.822(11)	$C^{(145)}$	$C^{(146)}$	1.383(14)
$P^{(2)}$	$N^{(1)}$	1.707(9)	$C^{(161)}$	$C^{(160)}$	1.402(16)
$P^{(2)}$	$C^{(14)}$	1.817(11)	$C^{(161)}$	$C^{(156)}$	1.391(15)
$P^{(2)}$	$C^{(8)}$	1.820(11)	$C^{(63)}$	$C^{(58)}$	1.417(17)
$P^{(8)}$	$N^{(4)}$	1.726(9)	$C^{(140)}$	$C^{(141)}$	1.370(19)

Table 4 Bond Lengths for marco1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P(8)	C(144)	1.799(10)	C(4)	C(3)	1.406(14)
P(8)	C(138)	1.793(10)	C(112)	C(107)	1.396(15)
P(4)	N(2)	1.709(8)	C(14)	C(20)	1.413(15)
P(4)	C(52)	1.796(11)	C(14)	C(15)	1.377(15)
P(4)	C(58)	1.821(11)	C(51)	C(50)	1.400(17)
P(5)	N(3)	1.708(9)	C(113)	C(118)	1.392(15)
P(5)	C(125)	1.820(11)	C(113)	C(114)	1.432(15)
P(5)	C(119)	1.817(12)	C(108)	C(107)	1.376(15)
P(6)	N(3)	1.716(9)	C(108)	C(109)	1.386(16)
P(6)	C(113)	1.813(11)	C(20)	C(18)	1.408(14)
P(6)	C(107)	1.821(11)	C(54)	C(55)	1.395(15)
P(1)	N(1)	1.739(9)	C(45)	C(44)	1.400(16)
P(1)	C(27)	1.822(10)	C(45)	C(40)	1.369(15)
P(1)	C(21)	1.796(11)	C(116)	C(115)	1.395(18)
S(1)	C(4)	1.754(9)	C(116)	C(117)	1.378(18)
S(1)	C(7)	1.790(11)	C(127)	C(128)	1.401(19)
S(4)	C(135)	1.755(9)	C(115)	C(114)	1.368(15)
S(4)	C(137)	1.765(13)	C(150)	C(151)	1.410(16)
S(3)	C(103)	1.756(11)	C(150)	C(155)	1.352(16)
S(3)	C(106)	1.811(16)	C(44)	C(43)	1.391(19)
S(2)	C(36)	1.770(11)	C(12)	C(11)	1.367(18)
S(2)	C(39)	1.802(14)	C(154)	C(155)	1.422(15)
N(1)	C(1)	1.414(12)	C(24)	C(23)	1.391(17)
N(3)	C(100)	1.441(13)	C(41)	C(40)	1.392(16)
N(4)	C(132)	1.428(12)	C(55)	C(56)	1.392(16)
C(100)	C(101)	1.387(14)	C(30)	C(29)	1.35(2)
C(100)	C(105)	1.393(14)	C(30)	C(31)	1.44(2)
N(2)	C(33)	1.442(12)	C(61)	C(60)	1.400(19)
C(125)	C(126)	1.396(15)	C(160)	C(159)	1.380(15)
C(125)	C(130)	1.402(16)	C(151)	C(152)	1.371(19)
C(26)	C(25)	1.393(15)	C(146)	C(147)	1.387(18)
C(26)	C(21)	1.382(15)	C(118)	C(117)	1.410(15)
C(42)	C(41)	1.373(16)	C(158)	C(159)	1.40(2)
C(42)	C(43)	1.376(16)	C(158)	C(157)	1.397(18)
C(33)	C(34)	1.389(14)	C(3)	C(2)	1.387(13)
C(33)	C(38)	1.380(14)	C(119)	C(124)	1.383(16)
C(53)	C(54)	1.396(15)	C(147)	C(148)	1.391(19)
C(53)	C(52)	1.387(14)	C(57)	C(52)	1.398(16)
C(47)	C(46)	1.414(15)	C(57)	C(56)	1.378(16)
C(47)	C(48)	1.383(16)	C(104)	C(105)	1.378(15)
C(49)	C(50)	1.358(17)	C(104)	C(103)	1.379(15)
C(49)	C(48)	1.400(17)	C(34)	C(35)	1.380(15)
C(120)	C(121)	1.392(16)	C(23)	C(22)	1.389(16)
C(120)	C(119)	1.399(14)	C(10)	C(11)	1.392(17)
C(139)	C(138)	1.408(15)	C(58)	C(59)	1.400(17)
C(139)	C(140)	1.379(16)	C(32)	C(31)	1.380(15)
C(144)	C(145)	1.422(14)	C(38)	C(37)	1.403(15)
C(144)	C(149)	1.382(15)	C(128)	C(129)	1.39(2)
C(134)	C(135)	1.404(13)	C(101)	C(102)	1.386(15)
C(134)	C(133)	1.373(13)	C(102)	C(103)	1.427(15)
C(138)	C(143)	1.425(14)	C(148)	C(149)	1.395(15)
C(111)	C(112)	1.365(17)	C(109)	C(110)	1.403(17)
C(111)	C(110)	1.383(16)	C(37)	C(36)	1.401(15)
C(27)	C(28)	1.395(16)	C(130)	C(129)	1.374(17)
C(27)	C(32)	1.412(16)	C(35)	C(36)	1.396(15)
C(1)	C(6)	1.393(14)	C(59)	C(60)	1.378(16)
C(1)	C(2)	1.410(13)	C(15)	C(16)	1.395(15)
C(132)	C(133)	1.394(13)	C(156)	C(157)	1.387(15)

Table 5 Bond Angles for marco1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P(3)	Au(1)	P(1)	130.77(8)	C(133)	C(132)	C(131)	118.1(9)
P(2)	Au(1)	P(3)	131.87(9)	C(131)	C(132)	N(4)	120.3(9)
P(2)	Au(1)	P(1)	69.78(8)	C(26)	C(25)	C(24)	119.4(10)
P(4)	Au(1)	P(3)	69.70(8)	C(141)	C(142)	C(143)	120.1(11)
P(4)	Au(1)	P(2)	134.38(9)	C(10)	C(9)	C(8)	118.2(10)
P(4)	Au(1)	P(1)	132.15(8)	C(16)	C(17)	C(18)	121.6(11)
P(7)	Au(2)	P(8)	69.70(8)	C(63)	C(62)	C(61)	121.1(14)
P(7)	Au(2)	P(6)	133.35(9)	C(127)	C(126)	C(125)	120.9(12)
P(8)	Au(2)	P(6)	129.29(9)	C(29)	C(28)	C(27)	120.4(12)
P(5)	Au(2)	P(7)	135.91(9)	C(47)	C(46)	P(3)	117.4(8)
P(5)	Au(2)	P(8)	130.55(9)	C(51)	C(46)	P(3)	119.7(8)
P(5)	Au(2)	P(6)	69.66(8)	C(51)	C(46)	C(47)	121.7(10)
F(6)	P(100)	F(1)	88.7(3)	C(12)	C(13)	C(8)	119.3(12)
F(6)	P(100)	F(5)	89.2(4)	C(134)	C(135)	S(4)	127.1(8)
F(5)	P(100)	F(1)	89.6(4)	C(134)	C(135)	C(136)	117.4(8)
F(2)	P(100)	F(1)	90.4(4)	C(136)	C(135)	S(4)	115.4(7)
F(2)	P(100)	F(6)	89.2(4)	C(122)	C(121)	C(120)	119.1(11)
F(2)	P(100)	F(5)	178.4(4)	C(26)	C(21)	P(1)	117.1(9)
F(3)	P(100)	F(1)	90.5(3)	C(26)	C(21)	C(22)	119.3(10)
F(3)	P(100)	F(6)	179.2(4)	C(22)	C(21)	P(1)	123.6(8)
F(3)	P(100)	F(5)	90.9(4)	C(19)	C(6)	C(1)	121.7(9)
F(3)	P(100)	F(2)	90.7(4)	C(142)	C(143)	C(138)	119.4(10)
F(3)	P(100)	F(4)	91.0(4)	C(124)	C(123)	C(122)	119.5(11)
F(4)	P(100)	F(1)	178.4(4)	C(6)	C(19)	C(4)	120.9(9)
F(4)	P(100)	F(6)	89.8(4)	C(131)	C(136)	C(135)	120.4(9)
F(4)	P(100)	F(5)	90.9(4)	C(154)	C(153)	C(152)	119.8(11)
F(4)	P(100)	F(2)	89.1(4)	C(146)	C(145)	C(144)	118.5(10)
F(10)	P(101)	F(12)	90.7(3)	C(160)	C(161)	P(7)	116.8(8)
F(10)	P(101)	F(9)	91.5(3)	C(156)	C(161)	P(7)	123.8(8)
F(10)	P(101)	F(7)	178.7(4)	C(156)	C(161)	C(160)	119.1(10)
F(10)	P(101)	F(8)	91.7(4)	C(62)	C(63)	C(58)	120.0(12)
F(10)	P(101)	F(11)	90.5(4)	C(141)	C(140)	C(139)	119.9(11)
F(9)	P(101)	F(12)	177.8(4)	C(19)	C(4)	S(1)	115.8(7)
F(9)	P(101)	F(7)	89.8(3)	C(3)	C(4)	S(1)	126.6(7)
F(9)	P(101)	F(8)	90.6(4)	C(3)	C(4)	C(19)	117.6(8)
F(9)	P(101)	F(11)	89.8(4)	C(111)	C(112)	C(107)	120.9(10)
F(7)	P(101)	F(12)	88.0(3)	C(134)	C(133)	C(132)	120.6(9)
F(8)	P(101)	F(12)	89.7(4)	C(20)	C(14)	P(2)	117.6(8)
F(8)	P(101)	F(7)	88.3(4)	C(15)	C(14)	P(2)	121.7(8)
F(11)	P(101)	F(12)	89.8(4)	C(15)	C(14)	C(20)	120.0(10)
F(11)	P(101)	F(7)	89.5(4)	C(46)	C(51)	C(50)	116.4(11)
F(11)	P(101)	F(8)	177.7(4)	C(118)	C(113)	P(6)	121.7(8)
N(2)	P(3)	Au(1)	91.6(3)	C(118)	C(113)	C(114)	118.8(10)
N(2)	P(3)	C(46)	108.5(4)	C(114)	C(113)	P(6)	118.4(8)
N(2)	P(3)	C(40)	107.4(4)	C(107)	C(108)	C(109)	120.2(11)
C(46)	P(3)	Au(1)	118.4(3)	C(18)	C(20)	C(14)	118.8(11)
C(40)	P(3)	Au(1)	123.5(4)	C(55)	C(54)	C(53)	118.7(10)
C(40)	P(3)	C(46)	105.2(5)	C(40)	C(45)	C(44)	120.1(11)
N(4)	P(7)	Au(2)	91.9(3)	C(117)	C(116)	C(115)	120.9(12)
N(4)	P(7)	C(161)	109.2(5)	C(126)	C(127)	C(128)	120.3(13)
N(4)	P(7)	C(155)	108.2(5)	C(114)	C(115)	C(116)	119.6(12)
C(161)	P(7)	Au(2)	121.0(3)	C(155)	C(150)	C(151)	120.7(11)
C(155)	P(7)	Au(2)	121.4(4)	C(43)	C(44)	C(45)	119.2(11)
C(155)	P(7)	C(161)	103.5(5)	C(11)	C(12)	C(13)	121.4(11)
N(1)	P(2)	Au(1)	92.5(3)	C(153)	C(154)	C(155)	119.2(11)
N(1)	P(2)	C(14)	109.8(5)	C(23)	C(24)	C(25)	119.8(11)
N(1)	P(2)	C(8)	107.2(5)	C(9)	C(8)	P(2)	122.8(8)
C(14)	P(2)	Au(1)	119.6(4)	C(13)	C(8)	P(2)	116.7(8)
C(14)	P(2)	C(8)	104.2(5)	C(13)	C(8)	C(9)	120.4(10)
C(8)	P(2)	Au(1)	121.9(4)	C(42)	C(41)	C(40)	120.7(10)
N(4)	P(8)	Au(2)	91.6(3)	C(56)	C(55)	C(54)	119.9(11)
N(4)	P(8)	C(144)	108.4(5)	C(112)	C(107)	P(6)	116.1(8)

Table 5 Bond Angles for marco1.

N(4)	P(8)	C(138)	107.8(5)	C(108)	C(107)	P(6)	124.4(9)
C(144)	P(8)	Au(2)	118.1(3)	C(108)	C(107)	C(112)	119.5(10)
C(138)	P(8)	Au(2)	124.0(4)	C(29)	C(30)	C(31)	119.6(11)
C(138)	P(8)	C(144)	104.8(5)	C(62)	C(61)	C(60)	119.9(12)
N(2)	P(4)	Au(1)	92.0(3)	C(159)	C(160)	C(161)	121.6(12)
N(2)	P(4)	C(52)	107.8(4)	C(152)	C(151)	C(150)	119.3(11)
N(2)	P(4)	C(58)	108.8(4)	C(145)	C(146)	C(147)	122.0(12)
C(52)	P(4)	Au(1)	121.1(4)	C(113)	C(118)	C(117)	119.6(11)
C(52)	P(4)	C(58)	104.1(5)	C(115)	C(114)	C(113)	120.9(11)
C(58)	P(4)	Au(1)	121.1(4)	C(136)	C(131)	C(132)	121.8(9)
N(3)	P(5)	Au(2)	91.9(3)	C(17)	C(18)	C(20)	119.5(11)
N(3)	P(5)	C(125)	109.3(4)	C(159)	C(158)	C(157)	119.9(11)
N(3)	P(5)	C(119)	107.0(5)	C(2)	C(3)	C(4)	121.1(9)
C(125)	P(5)	Au(2)	119.2(4)	C(120)	C(119)	P(5)	115.4(9)
C(119)	P(5)	Au(2)	124.7(3)	C(124)	C(119)	P(5)	125.2(8)
C(119)	P(5)	C(125)	102.8(5)	C(124)	C(119)	C(120)	119.3(11)
N(3)	P(6)	Au(2)	91.1(3)	C(123)	C(124)	C(119)	121.1(11)
N(3)	P(6)	C(113)	107.8(5)	C(45)	C(40)	P(3)	124.1(9)
N(3)	P(6)	C(107)	107.1(5)	C(45)	C(40)	C(41)	119.8(10)
C(113)	P(6)	Au(2)	118.9(3)	C(41)	C(40)	P(3)	116.0(8)
C(113)	P(6)	C(107)	104.2(5)	C(146)	C(147)	C(148)	119.1(11)
C(107)	P(6)	Au(2)	125.2(4)	C(42)	C(43)	C(44)	120.5(11)
N(1)	P(1)	Au(1)	91.3(3)	C(56)	C(57)	C(52)	121.3(10)
N(1)	P(1)	C(27)	107.9(5)	C(105)	C(104)	C(103)	121.5(10)
N(1)	P(1)	C(21)	108.4(4)	C(35)	C(34)	C(33)	121.6(10)
C(27)	P(1)	Au(1)	117.3(3)	C(22)	C(23)	C(24)	120.4(10)
C(21)	P(1)	Au(1)	123.8(4)	C(11)	C(10)	C(9)	121.2(11)
C(21)	P(1)	C(27)	105.9(5)	C(53)	C(52)	P(4)	116.9(8)
C(4)	S(1)	C(7)	101.8(5)	C(53)	C(52)	C(57)	117.7(10)
C(135)	S(4)	C(137)	102.4(5)	C(57)	C(52)	P(4)	125.2(8)
C(103)	S(3)	C(106)	104.4(6)	C(160)	C(159)	C(158)	118.9(13)
C(36)	S(2)	C(39)	104.3(6)	C(3)	C(2)	C(1)	120.6(9)
P(2)	N(1)	P(1)	106.2(4)	C(150)	C(155)	P(7)	117.4(9)
C(1)	N(1)	P(2)	127.7(7)	C(150)	C(155)	C(154)	120.2(10)
C(1)	N(1)	P(1)	126.1(7)	C(154)	C(155)	P(7)	122.3(8)
P(5)	N(3)	P(6)	107.2(5)	C(63)	C(58)	P(4)	118.2(9)
C(100)	N(3)	P(5)	127.3(7)	C(59)	C(58)	P(4)	122.4(9)
C(100)	N(3)	P(6)	125.4(7)	C(59)	C(58)	C(63)	118.2(11)
P(7)	N(4)	P(8)	106.7(5)	C(31)	C(32)	C(27)	120.0(11)
C(132)	N(4)	P(7)	128.7(7)	C(151)	C(152)	C(153)	120.7(11)
C(132)	N(4)	P(8)	124.3(7)	C(33)	C(38)	C(37)	121.3(10)
C(101)	C(100)	N(3)	121.6(9)	C(140)	C(141)	C(142)	121.3(11)
C(101)	C(100)	C(105)	118.0(10)	C(116)	C(117)	C(118)	120.2(11)
C(105)	C(100)	N(3)	120.4(9)	C(129)	C(128)	C(127)	119.1(12)
P(4)	N(2)	P(3)	106.6(5)	C(30)	C(29)	C(28)	121.9(13)
C(33)	N(2)	P(3)	125.0(7)	C(102)	C(101)	C(100)	121.9(10)
C(33)	N(2)	P(4)	128.2(7)	C(101)	C(102)	C(103)	119.3(10)
C(126)	C(125)	P(5)	119.0(8)	C(147)	C(148)	C(149)	120.0(12)
C(126)	C(125)	C(130)	118.6(10)	C(23)	C(22)	C(21)	120.0(10)
C(130)	C(125)	P(5)	121.4(9)	C(121)	C(122)	C(123)	120.2(11)
C(21)	C(26)	C(25)	121.2(11)	C(57)	C(56)	C(55)	120.1(11)
C(41)	C(42)	C(43)	119.7(11)	C(108)	C(109)	C(110)	119.7(11)
C(34)	C(33)	N(2)	120.2(9)	C(104)	C(105)	C(100)	121.1(10)
C(38)	C(33)	N(2)	121.1(9)	C(36)	C(37)	C(38)	119.0(10)
C(38)	C(33)	C(34)	118.7(9)	C(129)	C(130)	C(125)	120.6(12)
C(52)	C(53)	C(54)	122.1(10)	C(34)	C(35)	C(36)	119.7(10)
C(48)	C(47)	C(46)	119.0(11)	C(60)	C(59)	C(58)	121.4(13)
C(50)	C(49)	C(48)	120.1(12)	C(130)	C(129)	C(128)	120.4(13)
C(121)	C(120)	C(119)	120.7(11)	C(111)	C(110)	C(109)	119.7(11)
C(140)	C(139)	C(138)	121.1(11)	C(49)	C(50)	C(51)	122.9(11)
C(145)	C(144)	P(8)	118.4(8)	C(144)	C(149)	C(148)	120.8(11)

Table 5 Bond Angles for marco1.

C(149)	C(144)	P(8)	121.3(8)	C(14)	C(15)	C(16)	120.9(11)
C(149)	C(144)	C(145)	119.5(9)	C(32)	C(31)	C(30)	119.1(12)
C(133)	C(134)	C(135)	121.7(10)	C(47)	C(48)	C(49)	119.7(12)
C(139)	C(138)	P(8)	119.1(8)	C(17)	C(16)	C(15)	119.1(12)
C(139)	C(138)	C(143)	118.1(10)	C(104)	C(103)	S(3)	117.2(8)
C(143)	C(138)	P(8)	122.6(8)	C(104)	C(103)	C(102)	118.2(9)
C(112)	C(111)	C(110)	120.0(11)	C(102)	C(103)	S(3)	124.6(8)
C(28)	C(27)	P(1)	119.1(9)	C(12)	C(11)	C(10)	119.4(11)
C(28)	C(27)	C(32)	119.1(9)	C(59)	C(60)	C(61)	119.4(12)
C(32)	C(27)	P(1)	120.8(8)	C(157)	C(156)	C(161)	119.7(11)
C(6)	C(1)	N(1)	120.2(9)	C(37)	C(36)	S(2)	124.4(9)
C(6)	C(1)	C(2)	117.9(9)	C(35)	C(36)	S(2)	115.9(8)
C(2)	C(1)	N(1)	121.9(9)	C(35)	C(36)	C(37)	119.7(10)
C(133)	C(132)	N(4)	121.6(9)	C(156)	C(157)	C(158)	120.7(11)

Table 6 Torsion Angles for marco1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Au(1)	P(3)	N(2)	P(4)	-2.4(4)	C(62)	C(61)	C(60)	C(59)	3.1(18)
Au(1)	P(3)	N(2)	C(33)	172.0(8)	C(126)	C(125)	C(130)	C(129)	3.0(17)
Au(1)	P(3)	C(46)	C(47)	54.7(9)	C(126)	C(127)	C(128)	C(129)	-2.9(18)
Au(1)	P(3)	C(46)	C(51)	-113.1(8)	C(28)	C(27)	C(32)	C(31)	3.0(15)
Au(1)	P(3)	C(40)	C(45)	-165.9(7)	C(46)	P(3)	N(2)	P(4)	118.3(5)
Au(1)	P(3)	C(40)	C(41)	18.4(10)	C(46)	P(3)	N(2)	C(33)	-67.3(9)
Au(1)	P(2)	N(1)	P(1)	-4.1(4)	C(46)	P(3)	C(40)	C(45)	53.7(10)
Au(1)	P(2)	N(1)	C(1)	176.1(8)	C(46)	P(3)	C(40)	C(41)	-122.0(8)
Au(1)	P(2)	C(14)	C(20)	-47.5(9)	C(46)	C(47)	C(48)	C(49)	1.3(17)
Au(1)	P(2)	C(14)	C(15)	122.8(8)	C(46)	C(51)	C(50)	C(49)	-0.8(17)
Au(1)	P(2)	C(8)	C(9)	154.7(8)	C(13)	C(12)	C(11)	C(10)	-0.3(18)
Au(1)	P(2)	C(8)	C(13)	-29.6(10)	C(135)	C(134)	C(133)	C(132)	2.1(17)
Au(1)	P(4)	N(2)	P(3)	2.4(4)	C(135)	C(136)	C(131)	C(132)	1.8(16)
Au(1)	P(4)	N(2)	C(33)	-171.7(8)	C(121)	C(120)	C(119)	P(5)	175.7(9)
Au(1)	P(4)	C(52)	C(53)	32.9(10)	C(121)	C(120)	C(119)	C(124)	0.3(16)
Au(1)	P(4)	C(52)	C(57)	-151.5(8)	C(21)	P(1)	N(1)	P(2)	130.5(5)
Au(1)	P(4)	C(58)	C(63)	36.4(9)	C(21)	P(1)	N(1)	C(1)	-49.7(10)
Au(1)	P(4)	C(58)	C(59)	-130.7(8)	C(21)	P(1)	C(27)	C(28)	168.7(8)
Au(1)	P(1)	N(1)	P(2)	4.1(4)	C(21)	P(1)	C(27)	C(32)	-23.5(10)
Au(1)	P(1)	N(1)	C(1)	-176.1(8)	C(21)	C(26)	C(25)	C(24)	-0.3(17)
Au(1)	P(1)	C(27)	C(28)	-48.4(9)	C(6)	C(1)	C(2)	C(3)	0.6(16)
Au(1)	P(1)	C(27)	C(32)	119.4(8)	C(6)	C(19)	C(4)	S(1)	-178.7(9)
Au(1)	P(1)	C(21)	C(26)	-17.8(10)	C(6)	C(19)	C(4)	C(3)	-1.2(17)
Au(1)	P(1)	C(21)	C(22)	163.3(7)	C(143)	C(142)	C(141)	C(140)	2.0(19)
Au(2)	P(7)	N(4)	P(8)	-3.1(4)	C(19)	C(4)	C(3)	C(2)	-1.2(17)
Au(2)	P(7)	N(4)	C(132)	170.4(9)	C(153)	C(154)	C(155)	P(7)	176.3(9)
Au(2)	P(7)	C(161)	C(160)	-33.5(10)	C(153)	C(154)	C(155)	C(150)	-0.5(16)
Au(2)	P(7)	C(161)	C(156)	139.1(8)	C(145)	C(144)	C(149)	C(148)	0.7(15)
Au(2)	P(7)	C(155)	C(150)	-33.7(10)	C(145)	C(146)	C(147)	C(148)	0.5(17)
Au(2)	P(7)	C(155)	C(154)	149.3(7)	C(161)	P(7)	N(4)	P(8)	-127.0(5)
Au(2)	P(8)	N(4)	P(7)	3.1(4)	C(161)	P(7)	N(4)	C(132)	46.5(10)
Au(2)	P(8)	N(4)	C(132)	-170.8(8)	C(161)	P(7)	C(155)	C(150)	106.4(9)
Au(2)	P(8)	C(144)	C(145)	-57.4(8)	C(161)	P(7)	C(155)	C(154)	-70.5(10)
Au(2)	P(8)	C(144)	C(149)	112.5(8)	C(161)	C(160)	C(159)	C(158)	-0.7(18)
Au(2)	P(8)	C(138)	C(139)	-15.3(11)	C(161)	C(156)	C(157)	C(158)	-1.3(16)
Au(2)	P(8)	C(138)	C(143)	169.0(7)	C(63)	C(62)	C(61)	C(60)	-1.0(19)
Au(2)	P(5)	N(3)	P(6)	2.4(4)	C(63)	C(58)	C(59)	C(60)	2.4(16)
Au(2)	P(5)	N(3)	C(100)	-174.0(8)	C(140)	C(139)	C(138)	P(8)	-177.4(9)
Au(2)	P(5)	C(125)	C(126)	44.4(9)	C(140)	C(139)	C(138)	C(143)	-1.4(16)
Au(2)	P(5)	C(125)	C(130)	-123.5(9)	C(4)	C(3)	C(2)	C(1)	1.4(17)
Au(2)	P(5)	C(119)	C(120)	32.5(10)	C(112)	C(111)	C(110)	C(109)	1.0(18)
Au(2)	P(5)	C(119)	C(124)	-152.5(8)	C(133)	C(134)	C(135)	S(4)	175.3(9)
Au(2)	P(6)	N(3)	P(5)	-2.4(4)	C(133)	C(134)	C(135)	C(136)	-1.0(16)

Table 6 Torsion Angles for marco1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Au(2)	P(6)	N(3)	C(100)	174.1(8)	C(133)	C(132)	C(131)	C(136)	-0.6(16)
Au(2)	P(6)	C(113)	C(118)	-119.7(8)	C(14)	P(2)	N(1)	P(1)	-126.9(5)
Au(2)	P(6)	C(113)	C(114)	48.0(10)	C(14)	P(2)	N(1)	C(1)	53.3(10)
Au(2)	P(6)	C(107)	C(112)	18.8(10)	C(14)	P(2)	C(8)	C(9)	-65.9(10)
Au(2)	P(6)	C(107)	C(108)	-163.4(8)	C(14)	P(2)	C(8)	C(13)	109.8(9)
P(3)	N(2)	C(33)	C(34)	-107.6(11)	C(14)	C(20)	C(18)	C(17)	-1.8(16)
P(3)	N(2)	C(33)	C(38)	72.3(13)	C(14)	C(15)	C(16)	C(17)	-1.8(17)
P(3)	C(46)	C(51)	C(50)	167.3(8)	C(113)	P(6)	N(3)	P(5)	118.5(5)
P(7)	N(4)	C(132)	C(133)	114.8(11)	C(113)	P(6)	N(3)	C(100)	-65.0(9)
P(7)	N(4)	C(132)	C(131)	-66.6(13)	C(113)	P(6)	C(107)	C(112)	-123.1(9)
P(7)	C(161)	C(160)	C(159)	171.5(9)	C(113)	P(6)	C(107)	C(108)	54.7(10)
P(7)	C(161)	C(156)	C(157)	-170.0(8)	C(113)	C(118)	C(117)	C(116)	1.5(18)
P(2)	N(1)	C(1)	C(6)	-67.3(13)	C(108)	C(109)	C(110)	C(111)	-2.5(18)
P(2)	N(1)	C(1)	C(2)	113.3(11)	C(20)	C(14)	C(15)	C(16)	1.6(16)
P(2)	C(14)	C(20)	C(18)	170.7(8)	C(54)	C(53)	C(52)	P(4)	175.6(9)
P(2)	C(14)	C(15)	C(16)	-168.5(8)	C(54)	C(53)	C(52)	C(57)	-0.4(16)
P(8)	N(4)	C(132)	C(133)	-72.7(13)	C(54)	C(55)	C(56)	C(57)	-3.6(19)
P(8)	N(4)	C(132)	C(131)	105.9(10)	C(45)	C(44)	C(43)	C(42)	-3(2)
P(8)	C(144)	C(145)	C(146)	170.0(8)	C(116)	C(115)	C(114)	C(113)	0.2(18)
P(8)	C(144)	C(149)	C(148)	-169.1(8)	C(127)	C(128)	C(129)	C(130)	3.4(18)
P(8)	C(138)	C(143)	C(142)	177.9(9)	C(115)	C(116)	C(117)	C(118)	-1.2(18)
P(4)	N(2)	C(33)	C(34)	65.6(13)	C(150)	C(151)	C(152)	C(153)	-0.7(19)
P(4)	N(2)	C(33)	C(38)	-114.5(11)	C(44)	C(45)	C(40)	P(3)	-179.2(9)
P(4)	C(58)	C(59)	C(60)	169.4(9)	C(44)	C(45)	C(40)	C(41)	-3.7(16)
P(5)	N(3)	C(100)	C(101)	-113.4(11)	C(12)	C(13)	C(8)	P(2)	-176.1(9)
P(5)	N(3)	C(100)	C(105)	67.1(13)	C(12)	C(13)	C(8)	C(9)	-0.3(17)
P(5)	C(125)	C(126)	C(127)	-170.7(9)	C(154)	C(153)	C(152)	C(151)	1.3(19)
P(5)	C(125)	C(130)	C(129)	170.9(9)	C(24)	C(23)	C(22)	C(21)	-1.4(17)
P(5)	C(119)	C(124)	C(123)	-175.2(9)	C(8)	P(2)	N(1)	P(1)	120.5(5)
P(6)	N(3)	C(100)	C(101)	70.8(13)	C(8)	P(2)	N(1)	C(1)	-59.3(10)
P(6)	N(3)	C(100)	C(105)	-108.7(10)	C(8)	P(2)	C(14)	C(20)	172.0(8)
P(6)	C(113)	C(118)	C(117)	166.6(9)	C(8)	P(2)	C(14)	C(15)	-17.6(10)
P(6)	C(113)	C(114)	C(115)	-167.9(9)	C(8)	C(9)	C(10)	C(11)	-1.7(17)
P(1)	N(1)	C(1)	C(6)	112.9(10)	C(8)	C(13)	C(12)	C(11)	-0.1(18)
P(1)	N(1)	C(1)	C(2)	-66.4(13)	C(41)	C(42)	C(43)	C(44)	1.2(19)
P(1)	C(27)	C(28)	C(29)	166.0(8)	C(107)	P(6)	N(3)	P(5)	-129.9(5)
P(1)	C(27)	C(32)	C(31)	-164.8(8)	C(107)	P(6)	N(3)	C(100)	46.6(9)
P(1)	C(21)	C(22)	C(23)	179.0(8)	C(107)	P(6)	C(113)	C(118)	25.2(10)
S(1)	C(4)	C(3)	C(2)	176.1(9)	C(107)	P(6)	C(113)	C(114)	-167.1(9)
S(4)	C(135)	C(136)	C(131)	-177.7(8)	C(107)	C(108)	C(109)	C(110)	2.7(18)
N(1)	P(2)	C(14)	C(20)	57.5(9)	C(61)	C(62)	C(63)	C(58)	-0.5(19)
N(1)	P(2)	C(14)	C(15)	-132.2(9)	C(160)	C(161)	C(156)	C(157)	2.5(15)
N(1)	P(2)	C(8)	C(9)	50.4(10)	C(151)	C(150)	C(155)	P(7)	-175.9(9)
N(1)	P(2)	C(8)	C(13)	-133.9(9)	C(151)	C(150)	C(155)	C(154)	1.1(17)
N(1)	P(1)	C(27)	C(28)	52.7(9)	C(146)	C(147)	C(148)	C(149)	0.1(17)
N(1)	P(1)	C(27)	C(32)	-139.5(8)	C(118)	C(113)	C(114)	C(115)	0.1(17)
N(1)	P(1)	C(21)	C(26)	-122.4(8)	C(114)	C(113)	C(118)	C(117)	-1.0(16)
N(1)	P(1)	C(21)	C(22)	58.7(10)	C(131)	C(132)	C(133)	C(134)	-1.3(16)
N(1)	C(1)	C(6)	C(19)	177.7(10)	C(18)	C(17)	C(16)	C(15)	0.2(17)
N(1)	C(1)	C(2)	C(3)	180.0(10)	C(119)	P(5)	N(3)	P(6)	-124.9(5)
N(3)	P(5)	C(125)	C(126)	-59.3(10)	C(119)	P(5)	N(3)	C(100)	58.6(10)
N(3)	P(5)	C(125)	C(130)	132.8(9)	C(119)	P(5)	C(125)	C(126)	-172.7(9)
N(3)	P(5)	C(119)	C(120)	137.2(8)	C(119)	P(5)	C(125)	C(130)	19.4(10)
N(3)	P(5)	C(119)	C(124)	-47.7(11)	C(119)	C(120)	C(121)	C(122)	-1.8(17)
N(3)	P(6)	C(113)	C(118)	138.8(9)	C(124)	C(123)	C(122)	C(121)	-3.3(19)
N(3)	P(6)	C(113)	C(114)	-53.5(9)	C(40)	P(3)	N(2)	P(4)	-128.4(5)
N(3)	P(6)	C(107)	C(112)	122.9(8)	C(40)	P(3)	N(2)	C(33)	46.0(9)
N(3)	P(6)	C(107)	C(108)	-59.3(10)	C(40)	P(3)	C(46)	C(47)	-162.5(8)
N(3)	C(100)	C(101)	C(102)	179.8(10)	C(40)	P(3)	C(46)	C(51)	29.7(9)
N(3)	C(100)	C(105)	C(104)	-177.7(10)	C(40)	C(45)	C(44)	C(43)	4.4(18)
N(4)	P(7)	C(161)	C(160)	71.0(9)	C(147)	C(148)	C(149)	C(144)	-0.7(16)

Table 6 Torsion Angles for marco1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N(4)	P(7)	C(161)	C(156)	-116.3(9)	C(43)	C(42)	C(41)	C(40)	-0.4(18)
N(4)	P(7)	C(155)	C(150)	-137.7(9)	C(34)	C(33)	C(38)	C(37)	0.3(17)
N(4)	P(7)	C(155)	C(154)	45.4(10)	C(34)	C(35)	C(36)	S(2)	178.2(9)
N(4)	P(8)	C(144)	C(145)	44.8(9)	C(34)	C(35)	C(36)	C(37)	-1.2(17)
N(4)	P(8)	C(144)	C(149)	-145.3(8)	C(10)	C(9)	C(8)	P(2)	176.7(8)
N(4)	P(8)	C(138)	C(139)	-119.8(9)	C(10)	C(9)	C(8)	C(13)	1.2(16)
N(4)	P(8)	C(138)	C(143)	64.4(10)	C(52)	P(4)	N(2)	P(3)	-121.2(5)
N(4)	C(132)	C(133)	C(134)	177.3(10)	C(52)	P(4)	N(2)	C(33)	64.6(10)
N(4)	C(132)	C(131)	C(136)	-179.3(9)	C(52)	P(4)	C(58)	C(63)	177.2(8)
C(100)	C(101)	C(102)	C(103)	-1.9(17)	C(52)	P(4)	C(58)	C(59)	10.1(10)
N(2)	P(3)	C(46)	C(47)	-47.8(9)	C(52)	C(53)	C(54)	C(55)	-1.4(17)
N(2)	P(3)	C(46)	C(51)	144.5(8)	C(52)	C(57)	C(56)	C(55)	1.7(18)
N(2)	P(3)	C(40)	C(45)	-61.8(10)	C(159)	C(158)	C(157)	C(156)	-0.9(18)
N(2)	P(3)	C(40)	C(41)	122.5(8)	C(2)	C(1)	C(6)	C(19)	-3.0(16)
N(2)	P(4)	C(52)	C(53)	136.6(8)	C(155)	P(7)	N(4)	P(8)	120.9(5)
N(2)	P(4)	C(52)	C(57)	-47.7(10)	C(155)	P(7)	N(4)	C(132)	-65.6(10)
N(2)	P(4)	C(58)	C(63)	-68.0(9)	C(155)	P(7)	C(161)	C(160)	-173.9(8)
N(2)	P(4)	C(58)	C(59)	124.9(9)	C(155)	P(7)	C(161)	C(156)	-1.2(10)
N(2)	C(33)	C(34)	C(35)	-178.9(10)	C(155)	C(150)	C(151)	C(152)	-0.5(18)
N(2)	C(33)	C(38)	C(37)	-179.7(10)	C(58)	P(4)	N(2)	P(3)	126.4(5)
C(125)	P(5)	N(3)	P(6)	124.4(5)	C(58)	P(4)	N(2)	C(33)	-47.8(10)
C(125)	P(5)	N(3)	C(100)	-52.1(10)	C(58)	P(4)	C(52)	C(53)	-107.9(9)
C(125)	P(5)	C(119)	C(120)	-107.7(9)	C(58)	P(4)	C(52)	C(57)	67.8(10)
C(125)	P(5)	C(119)	C(124)	67.4(11)	C(58)	C(59)	C(60)	C(61)	-3.8(17)
C(125)	C(126)	C(127)	C(128)	2.4(18)	C(32)	C(27)	C(28)	C(29)	-2.0(15)
C(125)	C(130)	C(129)	C(128)	-3.6(19)	C(152)	C(153)	C(154)	C(155)	-0.7(17)
C(26)	C(25)	C(24)	C(23)	-0.9(18)	C(137)	S(4)	C(135)	C(134)	4.8(12)
C(26)	C(21)	C(22)	C(23)	0.2(16)	C(137)	S(4)	C(135)	C(136)	-178.9(10)
C(42)	C(41)	C(40)	P(3)	177.6(9)	C(38)	C(33)	C(34)	C(35)	1.1(17)
C(42)	C(41)	C(40)	C(45)	1.7(16)	C(38)	C(37)	C(36)	S(2)	-176.8(9)
C(33)	C(34)	C(35)	C(36)	-0.7(17)	C(38)	C(37)	C(36)	C(35)	2.5(17)
C(33)	C(38)	C(37)	C(36)	-2.1(17)	C(141)	C(142)	C(143)	C(138)	-2.4(17)
C(53)	C(54)	C(55)	C(56)	3.4(18)	C(117)	C(116)	C(115)	C(114)	0.3(18)
C(47)	C(46)	C(51)	C(50)	0.1(15)	C(29)	C(30)	C(31)	C(32)	1.3(17)
C(120)	C(121)	C(122)	C(123)	3.3(18)	C(101)	C(100)	C(105)	C(104)	2.8(16)
C(120)	C(119)	C(124)	C(123)	-0.3(17)	C(101)	C(102)	C(103)	S(3)	-176.6(9)
C(139)	C(138)	C(143)	C(142)	2.1(16)	C(101)	C(102)	C(103)	C(104)	2.4(16)
C(139)	C(140)	C(141)	C(142)	-1.3(18)	C(122)	C(123)	C(124)	C(119)	1.8(18)
C(144)	P(8)	N(4)	P(7)	-117.3(5)	C(56)	C(57)	C(52)	P(4)	-175.4(9)
C(144)	P(8)	N(4)	C(132)	68.8(9)	C(56)	C(57)	C(52)	C(53)	0.3(16)
C(144)	P(8)	C(138)	C(139)	124.8(9)	C(109)	C(108)	C(107)	P(6)	-179.2(9)
C(144)	P(8)	C(138)	C(143)	-50.9(10)	C(109)	C(108)	C(107)	C(112)	-1.5(17)
C(144)	C(145)	C(146)	C(147)	-0.5(16)	C(105)	C(100)	C(101)	C(102)	-0.7(16)
C(134)	C(135)	C(136)	C(131)	-1.0(15)	C(105)	C(104)	C(103)	S(3)	178.7(9)
C(138)	P(8)	N(4)	P(7)	129.7(5)	C(105)	C(104)	C(103)	C(102)	-0.3(16)
C(138)	P(8)	N(4)	C(132)	-44.2(10)	C(130)	C(125)	C(126)	C(127)	-2.4(17)
C(138)	P(8)	C(144)	C(145)	159.7(8)	C(110)	C(111)	C(112)	C(107)	0.2(17)
C(138)	P(8)	C(144)	C(149)	-30.4(10)	C(50)	C(49)	C(48)	C(47)	-2.0(17)
C(138)	C(139)	C(140)	C(141)	1.0(17)	C(149)	C(144)	C(145)	C(146)	-0.1(14)
C(111)	C(112)	C(107)	P(6)	177.9(9)	C(15)	C(14)	C(20)	C(18)	0.2(15)
C(111)	C(112)	C(107)	C(108)	0.0(16)	C(31)	C(30)	C(29)	C(28)	-0.2(18)
C(27)	P(1)	N(1)	P(2)	-115.2(5)	C(48)	C(47)	C(46)	P(3)	-167.9(8)
C(27)	P(1)	N(1)	C(1)	64.6(9)	C(48)	C(47)	C(46)	C(51)	-0.4(16)
C(27)	P(1)	C(21)	C(26)	122.0(8)	C(48)	C(49)	C(50)	C(51)	1.8(18)
C(27)	P(1)	C(21)	C(22)	-56.9(10)	C(16)	C(17)	C(18)	C(20)	1.6(17)
C(27)	C(28)	C(29)	C(30)	0.6(17)	C(103)	C(104)	C(105)	C(100)	-2.3(17)
C(27)	C(32)	C(31)	C(30)	-2.7(16)	C(156)	C(161)	C(160)	C(159)	-1.5(16)
C(1)	C(6)	C(19)	C(4)	3.3(17)	C(39)	S(2)	C(36)	C(37)	-7.2(12)
C(25)	C(26)	C(21)	P(1)	-178.3(8)	C(39)	S(2)	C(36)	C(35)	173.4(9)
C(25)	C(26)	C(21)	C(22)	0.6(16)	C(157)	C(158)	C(159)	C(160)	1.9(18)
C(25)	C(24)	C(23)	C(22)	1.8(18)	C(7)	S(1)	C(4)	C(19)	-173.6(10)

Table 6 Torsion Angles for marco1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
$C^{(9)}$	$C^{(10)}$	$C^{(11)}$	$C^{(12)}$	1.3(18)	$C^{(7)}$	$S^{(1)}$	$C^{(4)}$	$C^{(3)}$	9.1(13)
$C^{(62)}$	$C^{(63)}$	$C^{(58)}$	$P^{(4)}$	-167.8(9)	$C^{(106)}$	$S^{(3)}$	$C^{(103)}$	$C^{(104)}$	170.3(9)
$C^{(62)}$	$C^{(63)}$	$C^{(58)}$	$C^{(59)}$	-0.2(16)	$C^{(106)}$	$S^{(3)}$	$C^{(103)}$	$C^{(102)}$	-10.8(12)

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for marco1.

Atom	*x*	*y*	*z*	U(eq)
$H^{(26)}$	5412.44	7802.26	6514.85	21
$H^{(42)}$	6811.23	7018.37	4010.02	28
$H^{(53)}$	1811.59	7264.77	6592.4	22
$H^{(47)}$	5013.12	6325.2	7045.4	25
$H^{(49)}$	7959.59	6441.61	7726.16	33
$H^{(120)}$	1864.56	7137.94	1715.99	23
$H^{(139)}$	1629.29	7767.27	-257.69	26
$H^{(134)}$	3023.25	11048.78	-654.89	30
$H^{(111)}$	6948.34	7022.64	-906.77	26
$H^{(25)}$	6823.94	8014.87	7028.73	24
$H^{(142)}$	337.91	9841.33	-1617.72	37
$H^{(9)}$	1602.45	9738.66	4092.19	24
$H^{(17)}$	6435.88	8658.2	3253.1	30
$H^{(62)}$	1863.53	6463.82	4069.25	38
$H^{(126)}$	3282.34	6523.48	-197.42	20
$H^{(28)}$	934.14	8685.95	5660.7	29
$H^{(13)}$	1690	7771.05	4577.54	27
$H^{(121)}$	926.82	6852.22	2551.95	33
$H^{(6)}$	4317.31	9737.53	4696.42	21
$H^{(143)}$	1998.93	9618.36	-1024.97	25
$H^{(123)}$	2081.55	4901.7	2587.89	31
$H^{(19)}$	3936.7	10878.31	4350.97	23
$H^{(136)}$	188.7	10807.12	153.14	21
$H^{(153)}$	5397.25	10005.73	1456.21	38
$H^{(145)}$	5376.11	8742.74	36.26	20
$H^{(63)}$	3126.88	6545.71	4741.97	28
$H^{(140)}$	14.67	8005.62	-867.02	29
$H^{(112)}$	5784.98	7215.45	-185.46	22
$H^{(133)}$	3891.59	9926.76	-288.28	23
$H^{(51)}$	7702.75	6467.98	6048.18	27
$H^{(108)}$	7054.13	5307.98	765.22	23
$H^{(20)}$	5472.42	8526.3	4876.14	20
$H^{(54)}$	880.59	7079.46	7441.75	25
$H^{(45)}$	7068.24	5371.67	5746.24	22
$H^{(116)}$	8113.62	6163.13	2844.08	36
$H^{(127)}$	2088.28	6472.76	-914.71	36
$H^{(115)}$	6183.72	6215.12	2914.95	29
$H^{(150)}$	5444.2	7790.6	1680.07	26
$H^{(44)}$	8176.58	5131.19	4995.71	33
$H^{(12)}$	15.95	8019.69	4003.26	28
$H^{(154)}$	3927.06	9758.19	1017.34	27
$H^{(24)}$	6583.5	9087.72	7133.21	35
$H^{(41)}$	5649.25	7228.74	4732.8	22
$H^{(55)}$	932.17	5981.35	7954.39	33
$H^{(30)}$	-611.93	8735.98	7111.19	46
$H^{(61)}$	221.72	6154.55	4345.93	38
$H^{(160)}$	1197.87	8343.95	1067.57	32
$H^{(151)}$	6913.24	8038.64	2136.23	37
$H^{(146)}$	6901.61	8791.3	-533.99	32
$H^{(118)}$	7824.89	6249.51	1153.17	26
$H^{(114)}$	5073.26	6291.43	2112.17	24
$H^{(131)}$	1031.86	9678.59	471.62	20
$H^{(18)}$	6889.21	8569.69	4209.29	31
$H^{(158)}$	-86.55	8859.15	2466.25	36

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for marco1.

Atom	*x*	*y*	*z*	U(eq)
H(3)	934.21	11083.53	5097.71	27
H(124)	3002.9	5198.49	1760.2	29
H(147)	6829.09	8684.34	-1463.72	47
H(43)	8105.43	5981.49	4147.85	33
H(57)	2982.49	5286.91	6822.98	24
H(104)	4634.89	4149.2	516.41	19
H(34)	4159.5	5279.45	5359.77	21
H(23)	4964.14	9940.29	6698.51	30
H(10)	-111.59	9963.01	3539.39	32
H(159)	-272.97	8450.77	1674.17	42
H(2)	1269.99	9933.93	5389.25	23
H(32)	2704.45	8775.47	7047.26	31
H(152)	6869.33	9140.02	2030.05	39
H(13A)	1882.22	12087.87	-1245.22	93
H(13B)	2447.6	12181.79	-688.23	93
H(13C)	1398.11	12756	-1058.88	93
H(38)	5633.86	5115.57	6899.3	22
H(141)	-591.03	9023.6	-1552.91	37
H(117)	8924.97	6200.17	1973.82	38
H(128)	274.4	6326.33	-710.64	40
H(29)	-644.42	8694.73	6176.31	37
H(101)	5662.6	5044.89	1915.24	20
H(102)	6239.4	3898.09	2063.89	24
H(148)	5176.21	8539.8	-1841.5	33
H(22)	3539.68	9716.51	6204.92	28
H(122)	954.05	5736.66	2959.52	35
H(56)	2074.8	5089.92	7667.37	30
H(109)	8178.02	5092.94	21.93	30
H(105)	4171.24	5288.36	356.54	20
H(37)	6287.73	3955.71	7072.45	22
H(130)	955.38	6190.32	959.32	30
H(35)	4726.26	4132.44	5529.95	22
H(59)	1057.4	6022.12	5997.66	32
H(129)	-229.16	6121.12	244.58	44
H(110)	8180.07	5968.11	-804.43	27
H(50)	8739.91	6477.12	6863.78	38
H(149)	3616.3	8508.34	-1286.05	29
H(15)	3165.74	8768.81	3573.19	26
H(31)	1107.21	8751.41	7574.28	37
H(48)	6106.07	6328.3	7838.56	30
H(16)	4596.67	8754.91	2928.18	38
H(11)	-876.5	9100.24	3482	32
H(60)	-138.79	5878.6	5325.68	31
H(156)	2971.99	9127.02	1979.92	28
H(39A)	7446.22	2917.78	7033.22	57
H(39B)	7138.8	2226.95	7118.85	57
H(39C)	6394.1	2779.57	7391.89	57
H(157)	1524.27	9206.91	2606.61	39
H(7A)	352.36	12135.22	4623.66	88
H(7B)	739.1	12800.75	4548.97	88
H(7C)	1118.56	12203.51	5127.85	88
H(10A)	7357.42	2885.16	1974.06	69
H(10B)	7099.38	2187.45	2023.34	69
H(10C)	6360.4	2686.53	2349.13	69

6. References

(1) Daaoub, A.; Morris, J. M. F.; Béland, V. A.; Demay-Drouhard, P.; Hussein, A.; Higgins, S. J.; Sadeghi, H.; Nichols, R. J.; Vezzoli, A.; Baumgartner, T.; Sangtarash, S. Not So Innocent After All: Interfacial Chemistry Determines Charge-Transport Efficiency in Single-Molecule Junctions. *Angewandte Chemie International Edition* **2023**, *62* (24), e202302150. https://doi.org/10.1002/anie.202302150.

(2) Wu, C.; Qiao, X.; Robertson, C. M.; Higgins, S. J.; Cai, C.; Nichols, R. J.; Vezzoli, A. A Chemically Soldered Polyoxometalate Single-Molecule Transistor. *Angewandte Chemie International Edition* **2020**, *59* (29), 12029–12034. https://doi.org/10.1002/anie.202002174.

(3) Naghibi, S.; Sangtarash, S.; Kumar, V. J.; Wu, J.-Z.; Judd, M. M.; Qiao, X.; Gorenskaia, E.; Higgins, S. J.; Cox, N.; Nichols, R. J.; Sadeghi, H.; Low, P. J.; Vezzoli, A. Redox-Addressable Single-Molecule Junctions Incorporating a Persistent Organic Radical. *Angewandte Chemie International Edition* **2022**, *61* (23), e202116985. https://doi.org/10.1002/anie.202116985.

(4) Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2 : A Complete Structure Solution, Refinement and Analysis Program. *Journal of Applied Crystallography* **2009**, *42* (2), 339–341. https://doi.org/10.1107/S0021889808042726.

(5) Sheldrick, G. M. SHELXT - Integrated Space-Group and Crystal-Structure Determination. *Acta Crystallographica Section A: Foundations of Crystallography* **2015**, *71* (1), 3–8. https://doi.org/10.1107/S2053273314026370.

(6) Sheldrick, G. M. Crystal Structure Refinement with SHELXL. *Acta Crystallographica Section C: Structural Chemistry* **2015**, *71* (Md), 3–8. https://doi.org/10.1107/S2053229614024218.