

Supporting Information for:

Cyclo-tetrakis(μ-diphenylphosphido)-1,5-bis(tri-tert-butylphosphine)-tetracopper

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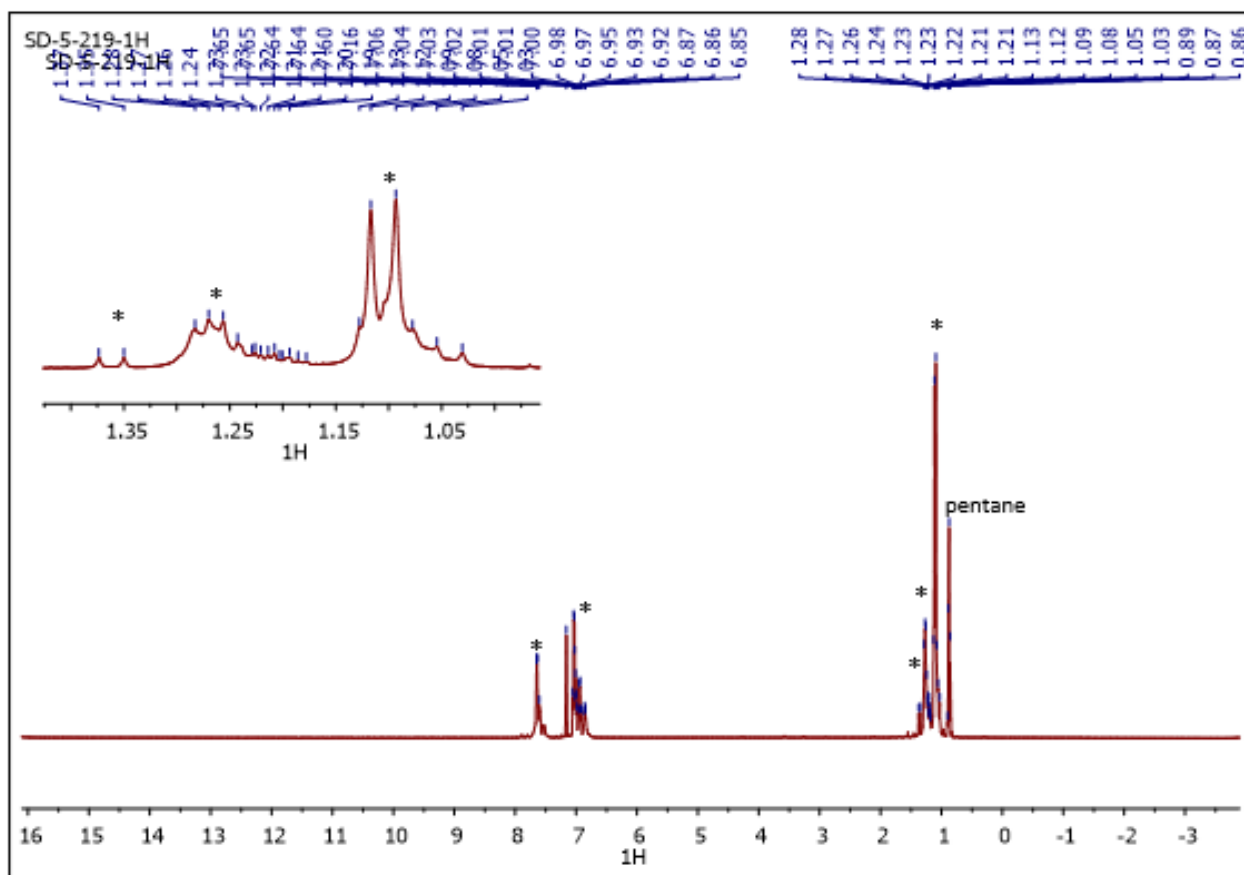
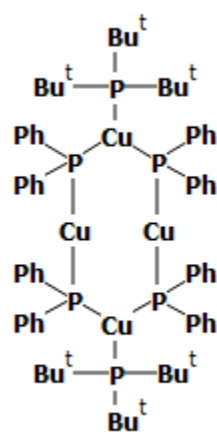


Figure S1. ^1H NMR spectra of **1** synthesized by method A (C_6D_6 , 500 MHz). Residual pentane is visible. * = signal for **1**.



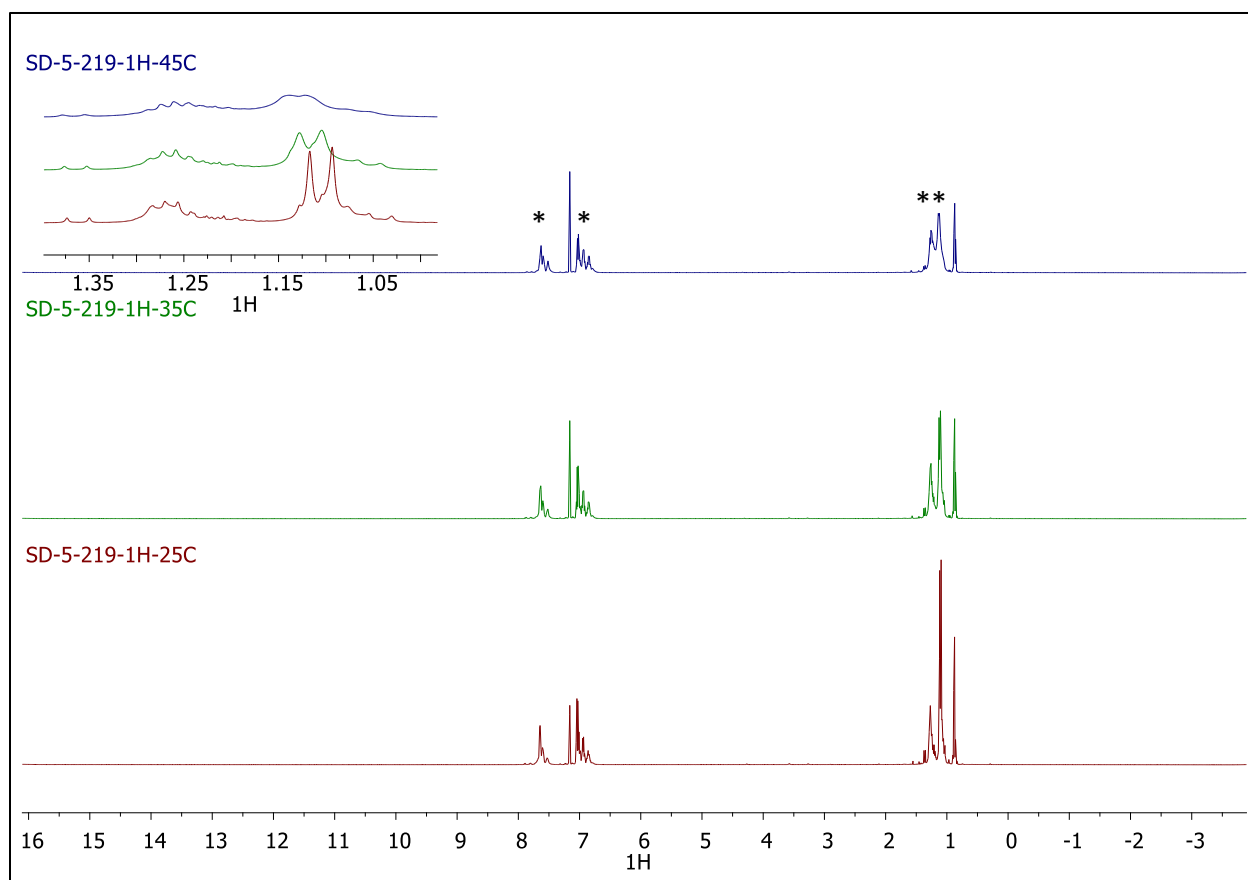
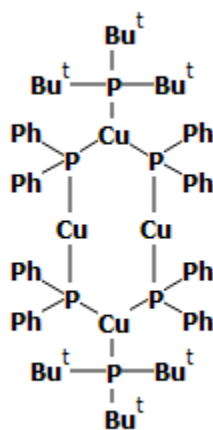


Figure S2. VT experiment - ^1H NMR spectra of **1** synthesized by method A (C_6D_6 , 500 MHz) at 25 °C (bottom) 35 °C (middle) 45 °C (top). * = signal for **1**.



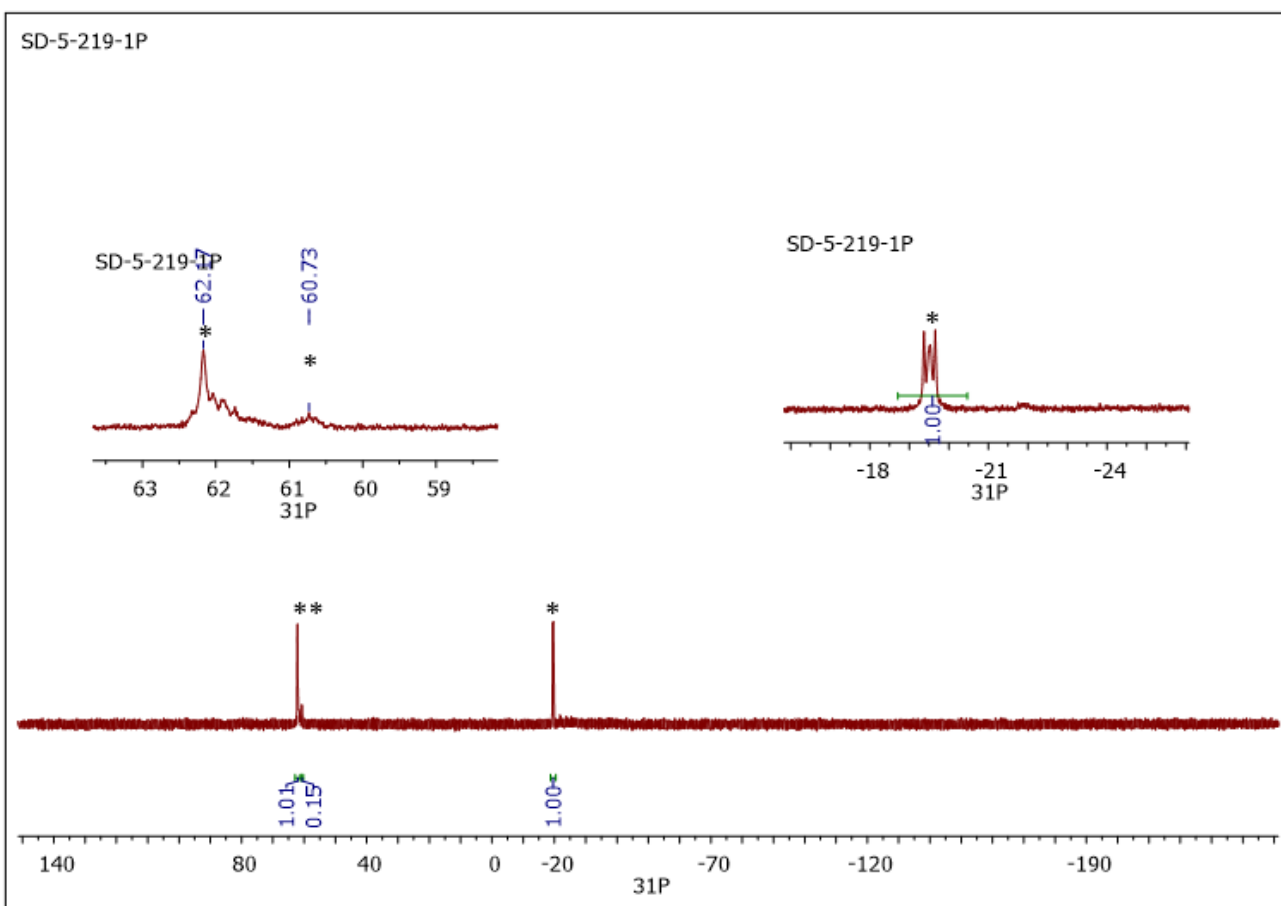
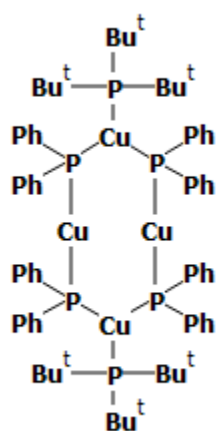


Figure S3. ^{31}P NMR spectra of **1** synthesized by method A (C_6D_6 , 202 MHz). * = signal for **1**.



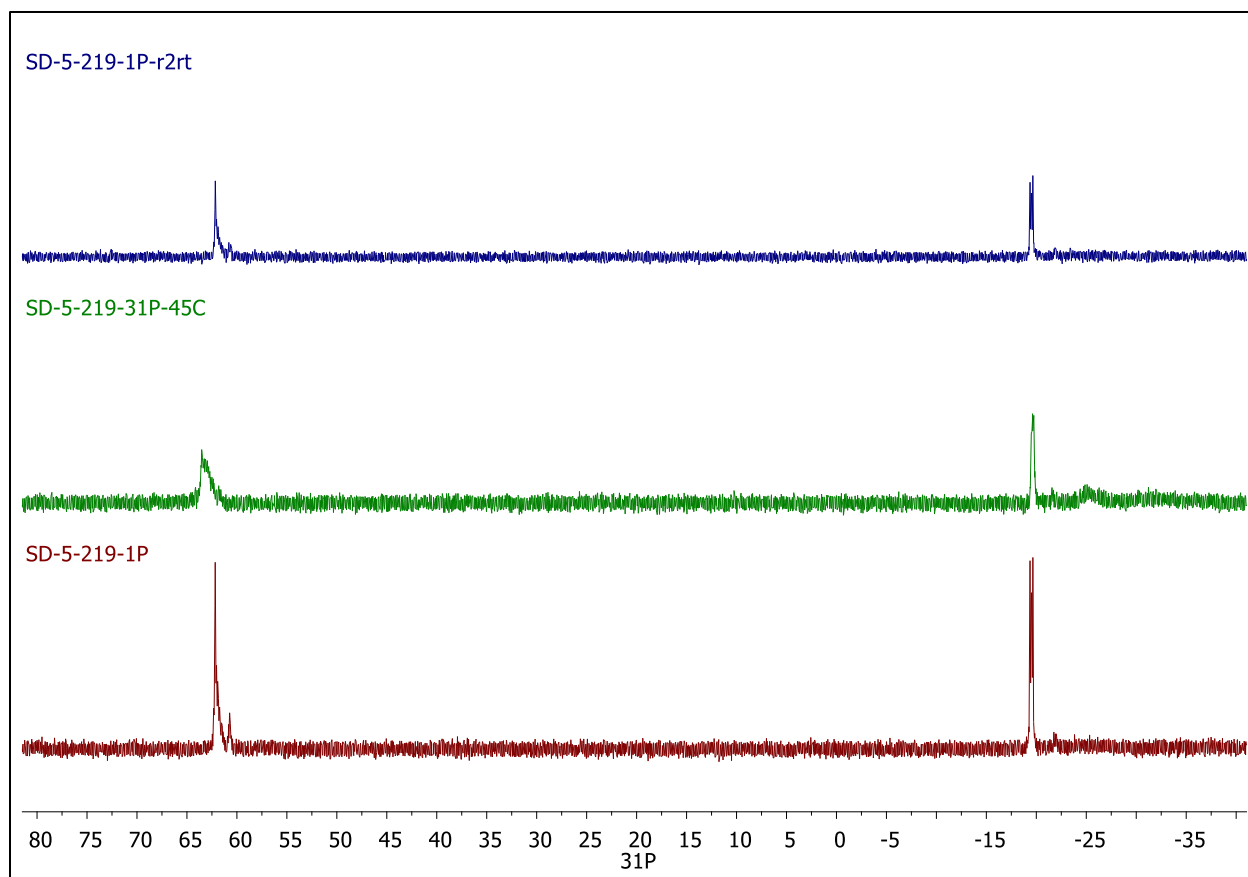
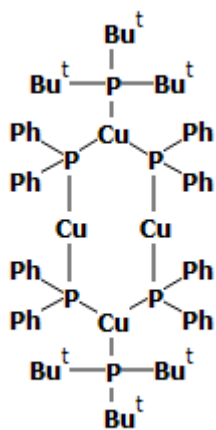


Figure S4. VT experiment - ^{31}P NMR spectra of **1** synthesized by method A at 25 °C (bottom) and 45 °C (middle), and upon returning to 25 °C (top).



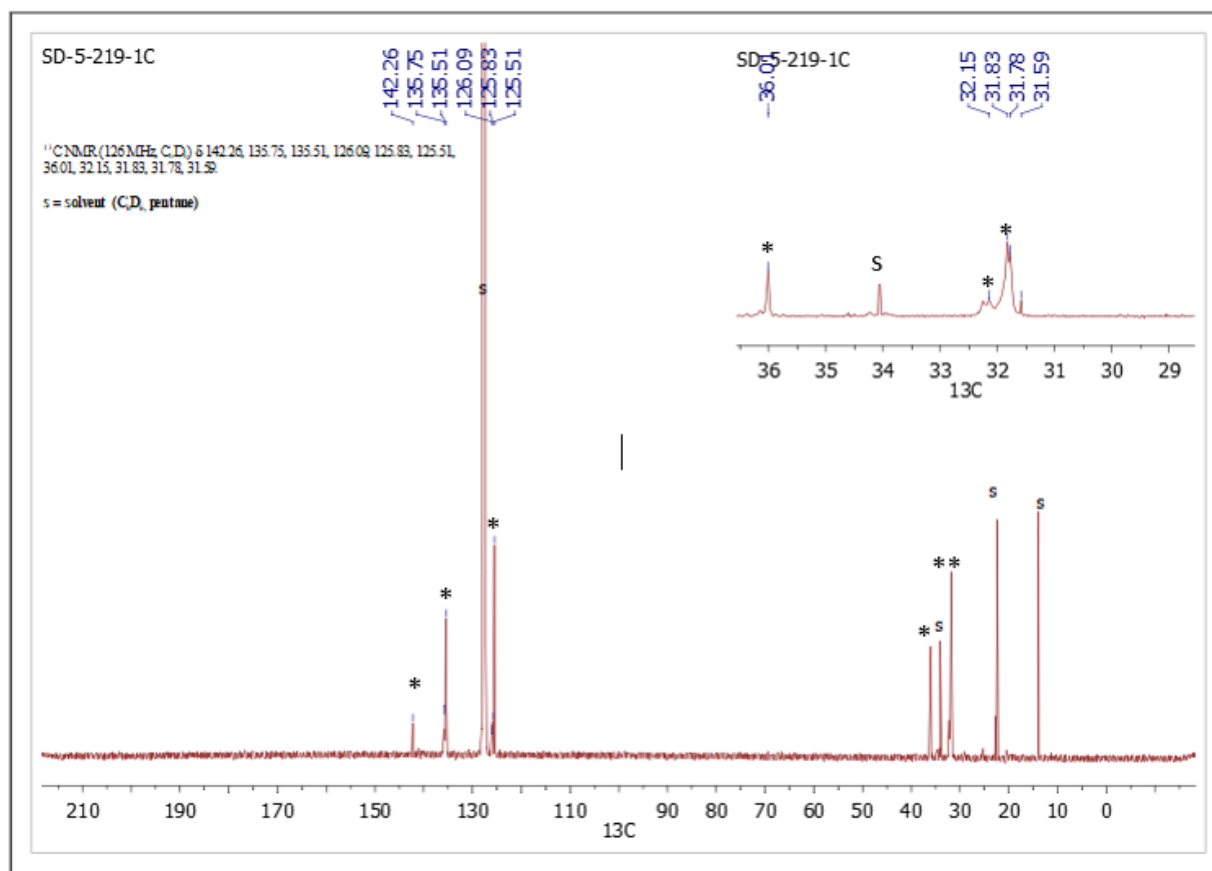
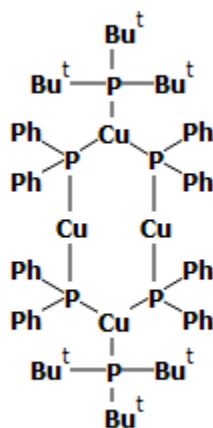


Figure S5. ^{13}C NMR spectra of **1** synthesized by method A (C_6D_6 , 126 MHz). Residual solvent is visible.

* = signal for **1**.



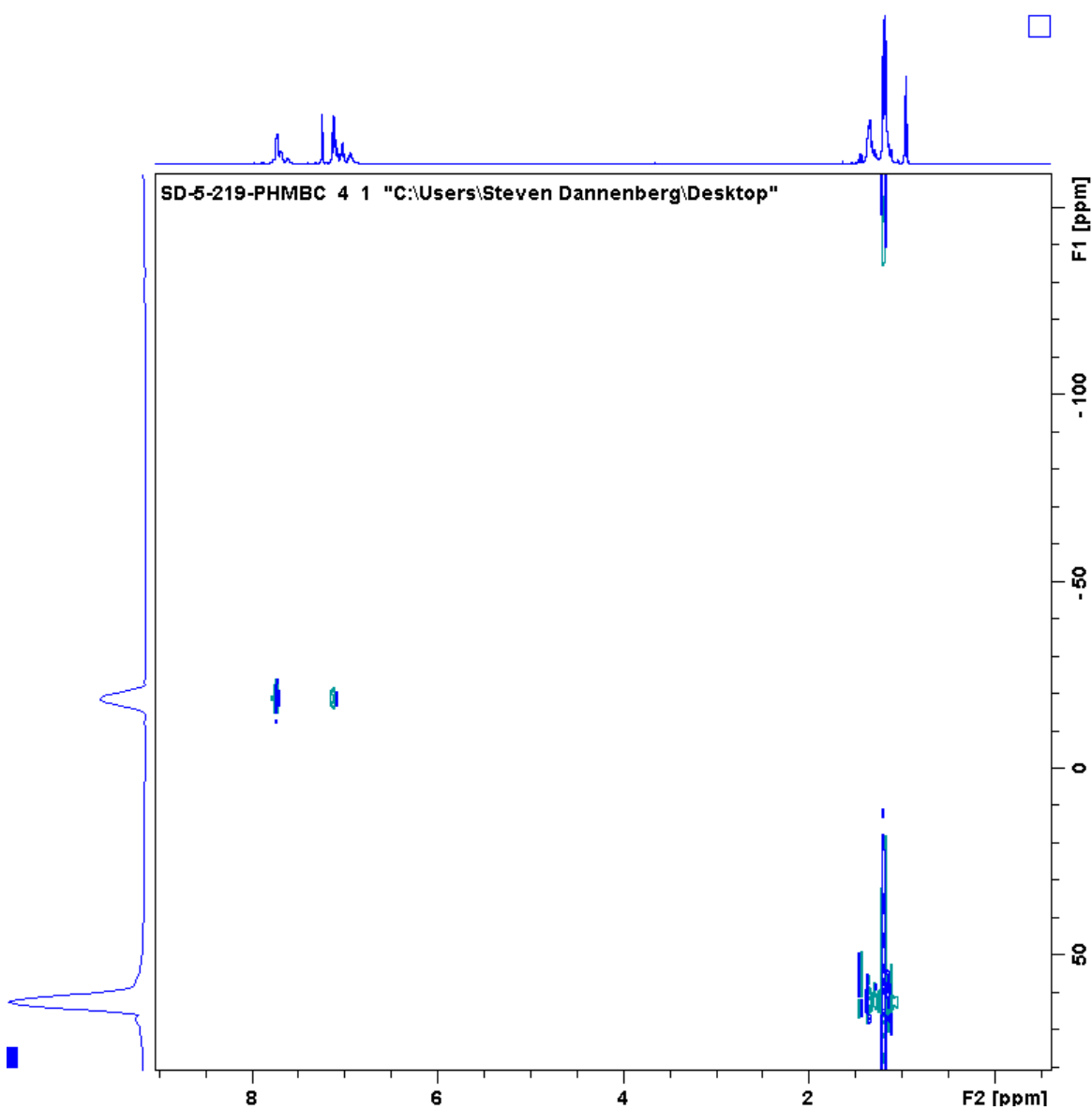
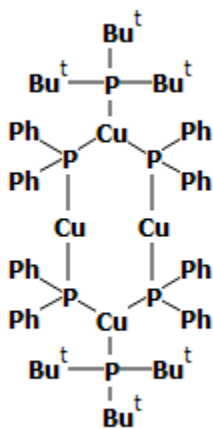


Figure S6. ^{31}P HMBC NMR spectrum of **1** synthesized by method A.



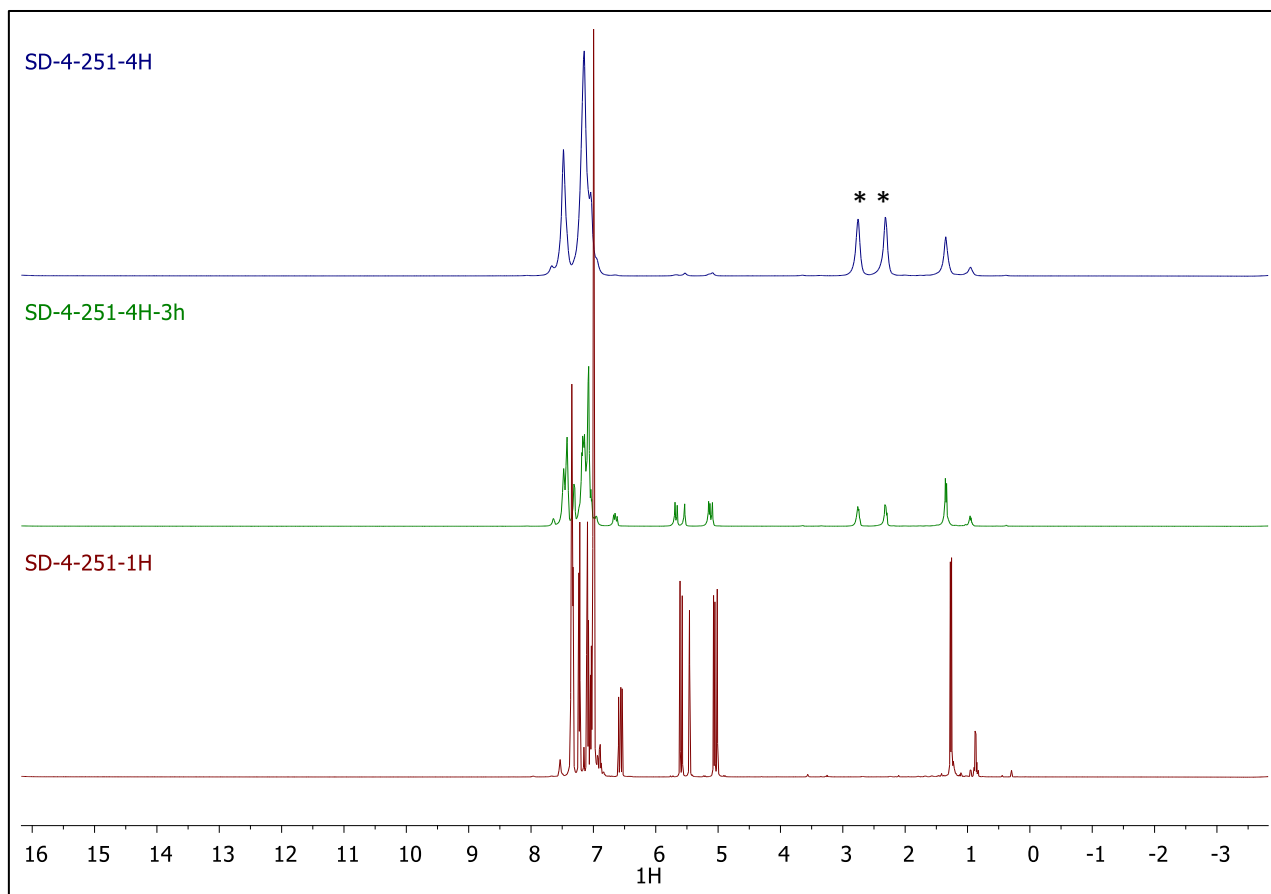
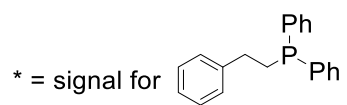


Figure S7. Stacked ¹H NMR spectra of the hydrophosphination of styrene with diphenylphosphine by 6 mol% of **1** under 360 nm irradiation. t = 0 (bottom), t = 3 h (middle), t = 24 h (top).



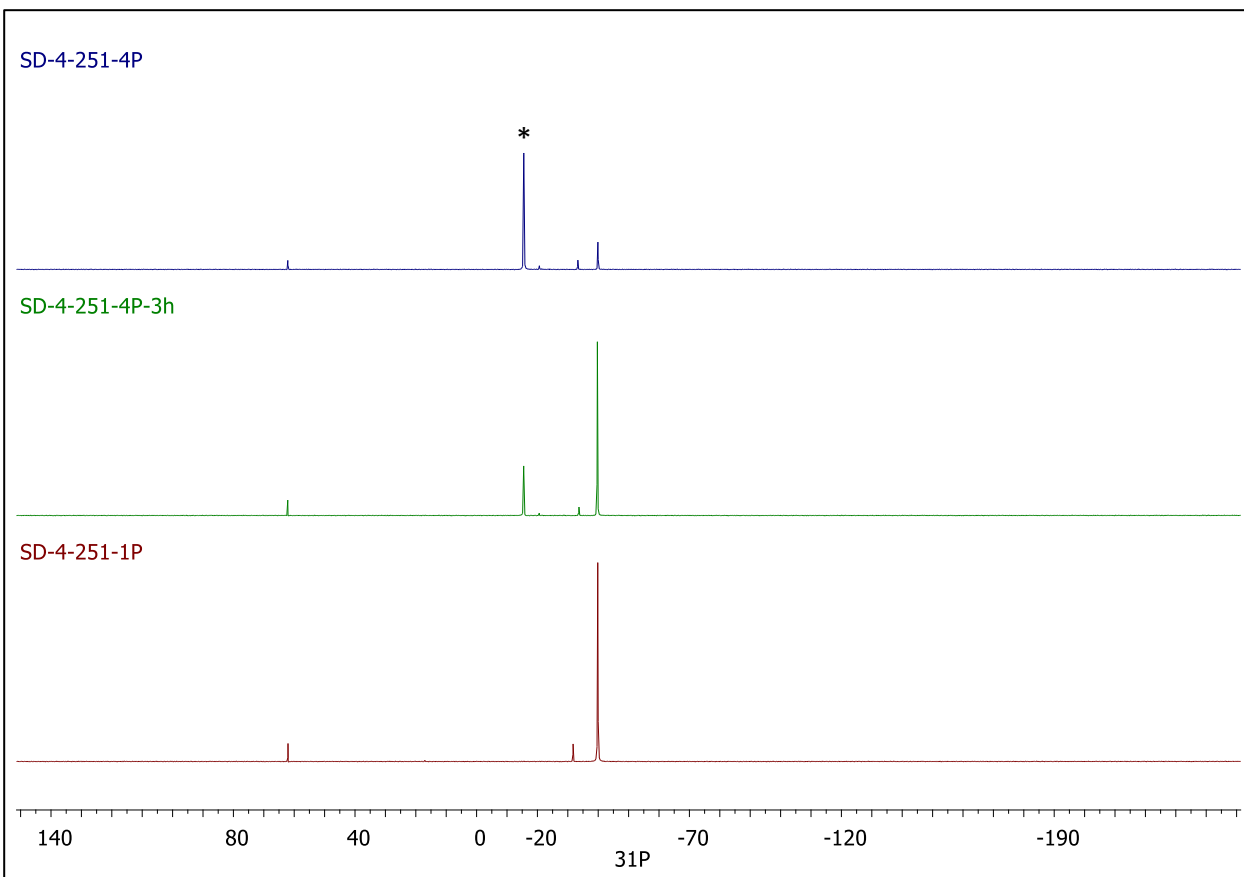
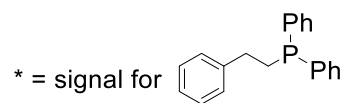


Figure S8. Stacked ^{31}P NMR spectra of the hydrophosphination of styrene with diphenylphosphine by 6 mol% of **1** under 360 nm irradiation. $t = 0$ (bottom), $t = 3$ h (middle), $t = 24$ h (top).



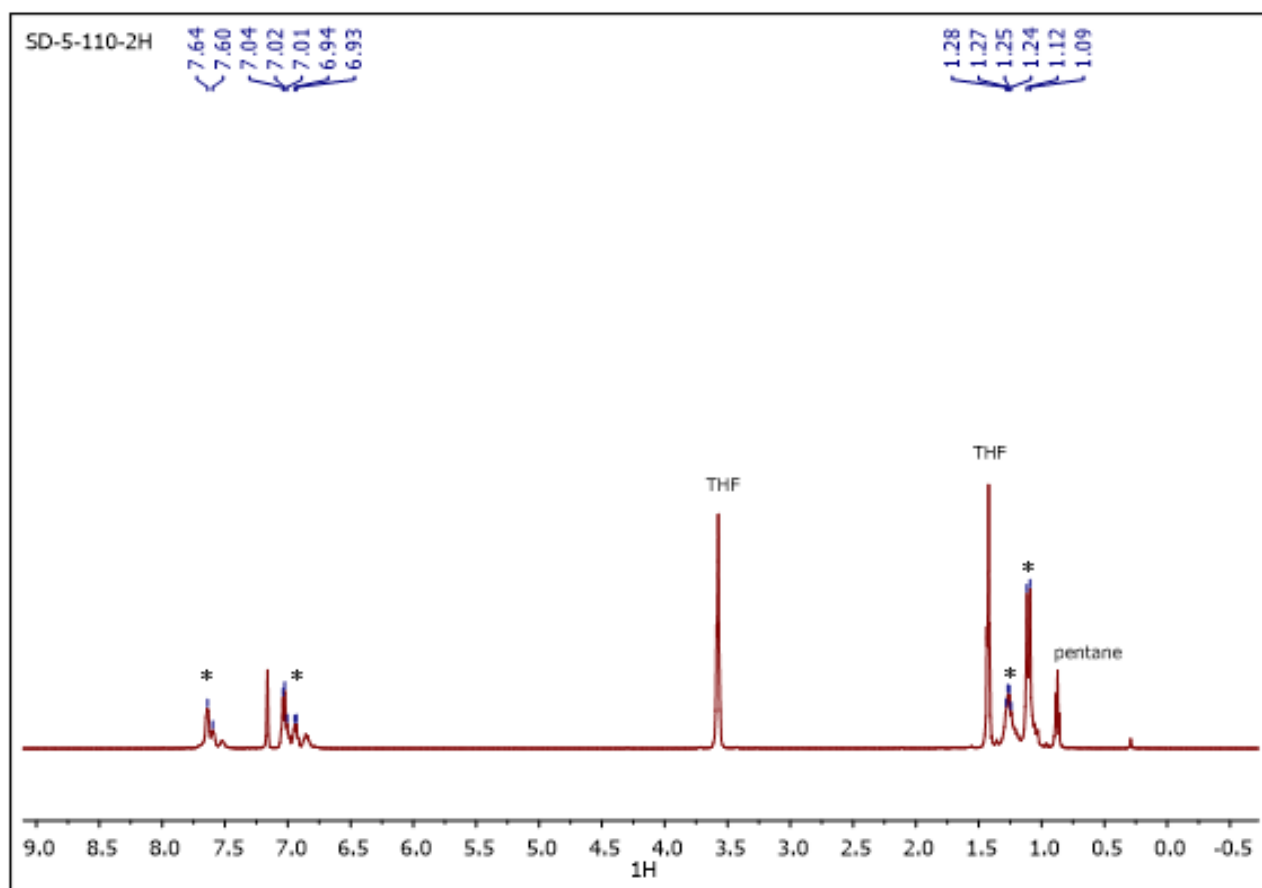
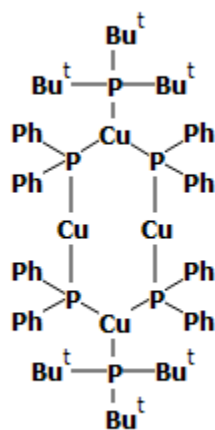


Figure S9. ^1H NMR spectra of **1** synthesized by method B (C_6D_6 $\delta = 7.16$, 500 MHz). Signal for residual THF and pentane is visible. * = signal for **1**.



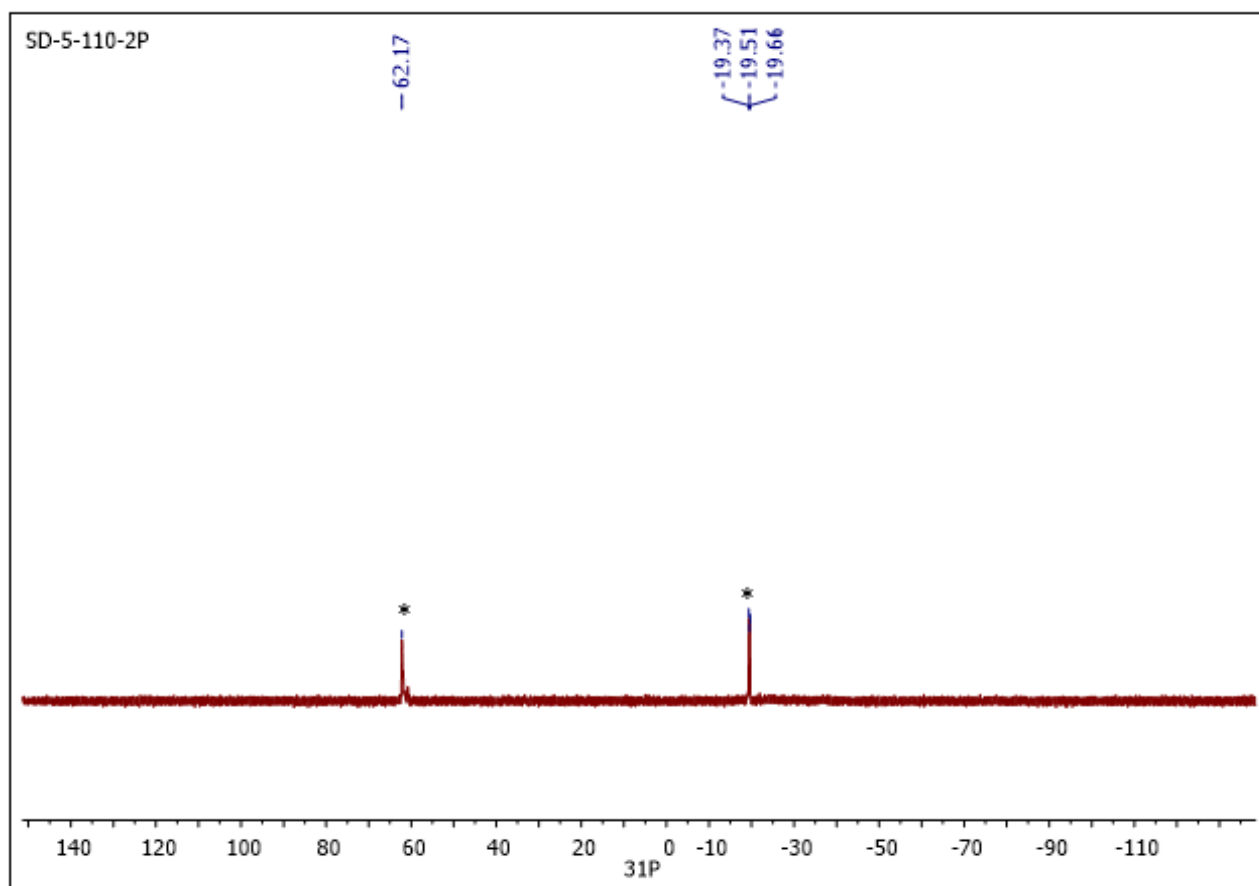
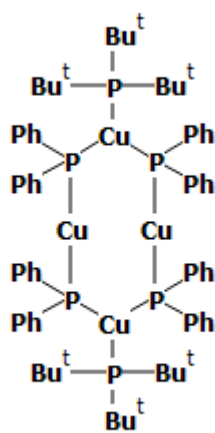


Figure S10. ^{31}P NMR spectra of **1** synthesized by method B (C_6D_6 , 202 MHz). * = signal for **1**.



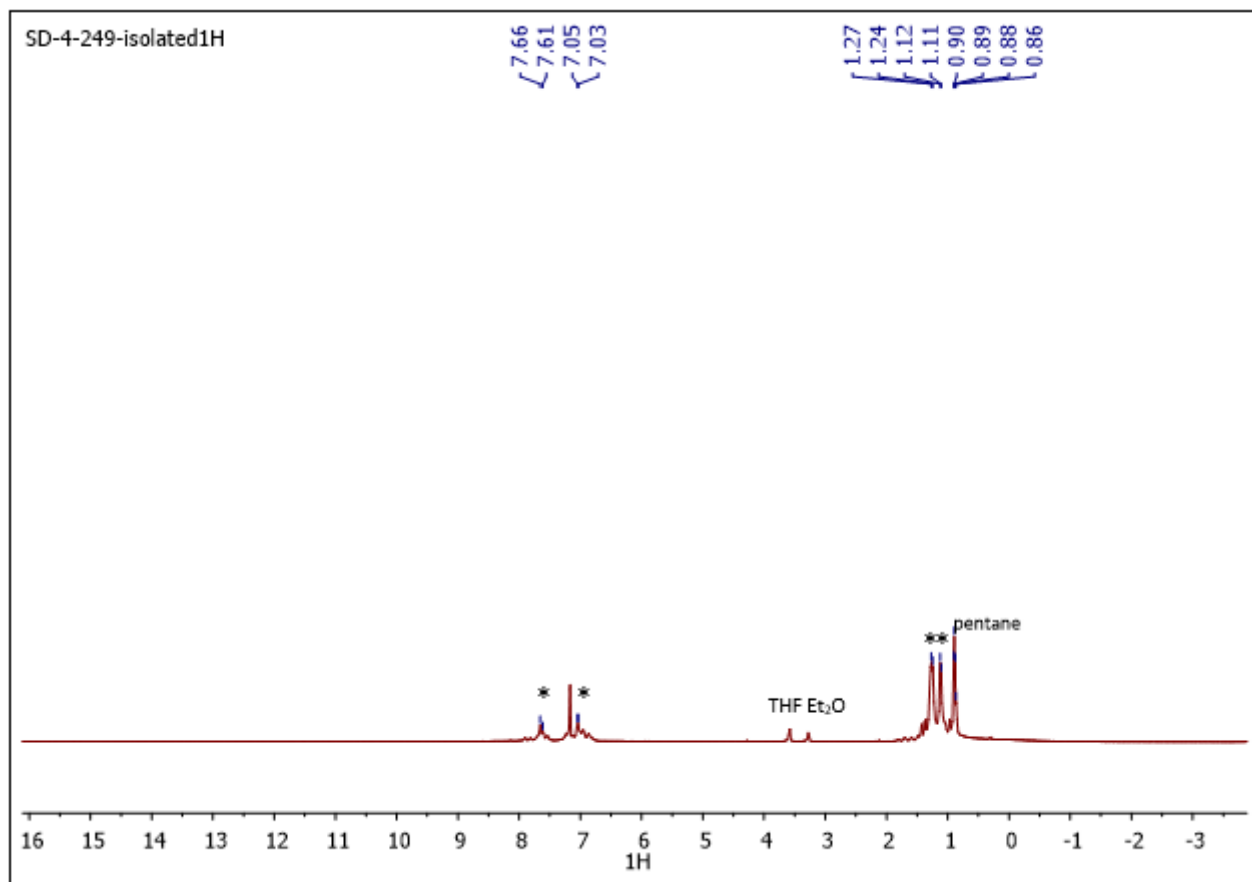
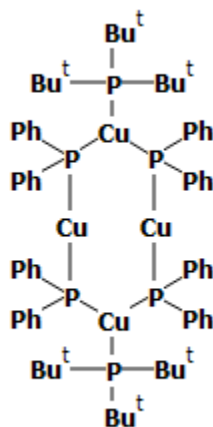


Figure S11. ¹H NMR spectra of **1** synthesized by method C (C₆D₆ δ = 7.16, 500 MHz). Residual solvent is visible and overlapping with alkyl peaks. * = signal for **1**.



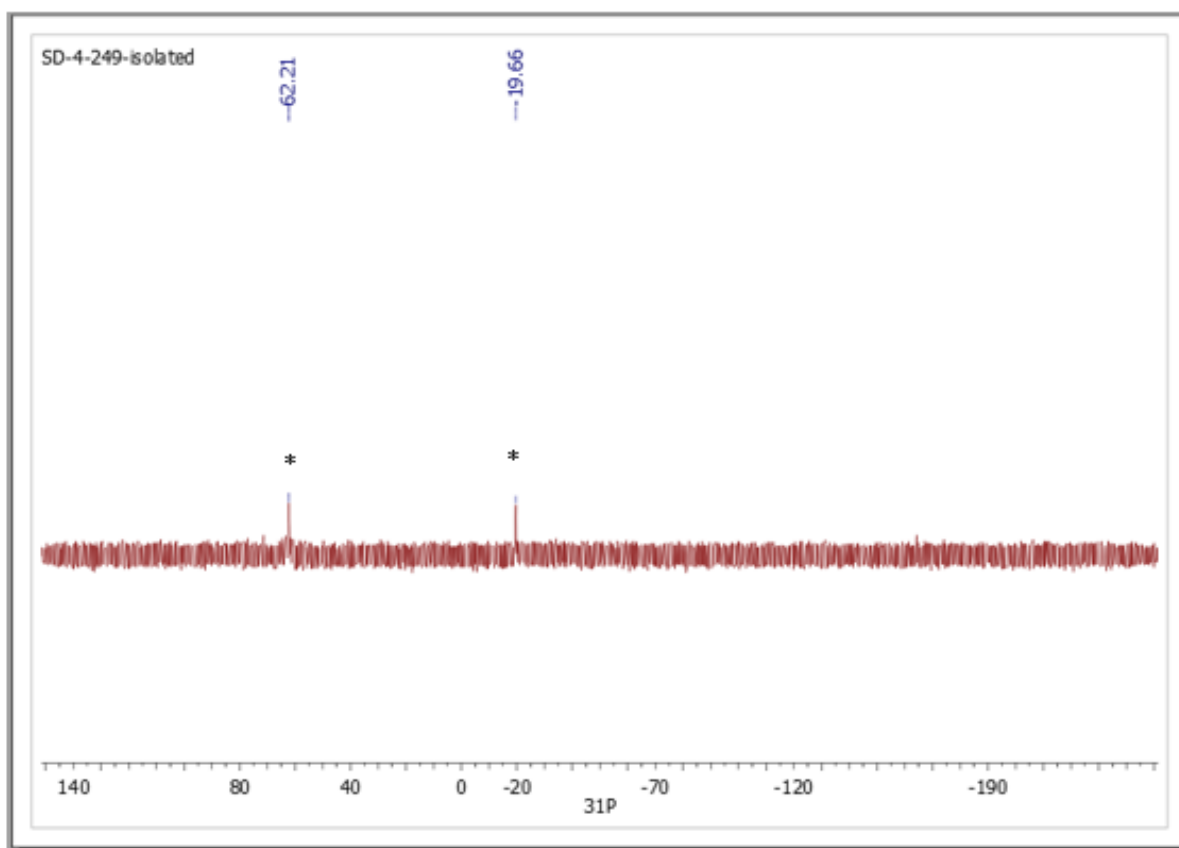


Figure S12. ^{31}P NMR spectra of **1** synthesized by method C (C_6D_6 , 202 MHz). * = signal for **1**.

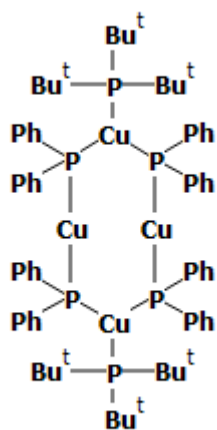


Figure S13. Bond Lengths and Angles

Atom-Atom	Length [Å]		
Cu1-P5	2.2738(10)	C14-H14	0.9500
Cu1-P4	2.3046(11)	C15-C16	1.370(4)
Cu1-P1	2.3076(10)	C15-H15	0.9500
P1-C19	1.844(2)	C16-C17	1.364(3)
P1-C25	1.848(2)	C16-H16	0.9500
P1-Cu2	2.2272(12)	C17-C18	1.384(3)
Cu2-P2	2.2209(13)	C17-H17	0.9500
Cu2-Cu4	2.8612(13)	C18-H18	0.9500
P2-C37	1.839(2)	C19-C24	1.384(3)
P2-C31	1.840(2)	C19-C20	1.387(3)
P2-Cu3	2.3047(11)	C20-C21	1.387(3)
Cu3-P6	2.2799(11)	C20-H20	0.9500
Cu3-P3	2.3068(10)	C21-C22	1.377(4)
P3-C72	1.840(2)	C21-H21	0.9500
P3-C1	1.840(2)	C22-C23	1.368(3)
P3-Cu4	2.2232(12)	C22-H22	0.9500
Cu4-P4	2.2273(12)	C24-C23	1.393(3)
P4-C7	1.839(2)	C24-H24	0.9500
P4-C13	1.842(2)	C23-H23	0.9500
P5-C55	1.903(2)	C25-C26	1.389(3)
P5-C59	1.903(2)	C25-C30	1.395(3)
P5-C63	1.907(2)	C26-C27	1.389(3)
P6-C47	1.907(2)	C26-H26	0.9500
P6-C52	1.909(2)	C27-C28	1.385(4)
P6-C43	1.914(2)	C27-H27	0.9500
C1-C2	1.376(3)	C28-C29	1.391(4)
C1-C6	1.390(3)	C28-H28	0.9500
C2-C3	1.389(4)	C29-C30	1.384(3)
C2-H2	0.9500	C29-H29	0.9500
C3-C4	1.363(5)	C30-H30	0.9500
C3-H3	0.9500	C31-C32	1.388(3)
C4-C5	1.373(5)	C31-C36	1.398(3)
C4-H4	0.9500	C32-C33	1.391(3)
C5-C6	1.389(4)	C32-H32	0.9500
C5-H5	0.9500	C33-C34	1.382(4)
C6-H6	0.9500	C33-H33	0.9500
C7-C12	1.397(3)	C34-C35	1.369(4)
C7-C8	1.397(3)	C34-H34	0.9500
C8-C9	1.383(3)	C35-C36	1.390(3)
C8-H8	0.9500	C35-H35	0.9500
C9-C10	1.380(4)	C36-H36	0.9500
C9-H9	0.9500	C37-C42	1.378(3)
C10-C11	1.382(4)	C37-C38	1.395(3)
C10-H10	0.9500	C38-C39	1.390(4)
C11-C12	1.392(3)	C38-H38	0.9500
C11-H11	0.9500	C39-C40	1.357(4)
C12-H12	0.9500	C39-H39	0.9500
C13-C14	1.383(3)	C40-C41	1.366(4)
C13-C18	1.393(3)	C40-H40	0.9500
C14-C15	1.391(3)	C41-C42	1.393(4)
		C41-H41	0.9500
		C42-H42	0.9500
		C43-C44	1.533(3)

C43-C45	1.543(3)	C61-H61A	0.9800
C43-C46	1.545(3)	C61-H61B	0.9800
C44-H44A	0.9800	C61-H61C	0.9800
C44-H44B	0.9800	C62-H62A	0.9800
C44-H44C	0.9800	C62-H62B	0.9800
C45-H45A	0.9800	C62-H62C	0.9800
C45-H45B	0.9800	C63-C66	1.516(4)
C45-H45C	0.9800	C63-C64	1.532(3)
C46-H46A	0.9800	C63-C65	1.551(3)
C46-H46B	0.9800	C64-H64A	0.9800
C46-H46C	0.9800	C64-H64B	0.9800
C47-C50	1.535(3)	C64-H64C	0.9800
C47-C48	1.544(3)	C65-H65A	0.9800
C47-C49	1.547(3)	C65-H65B	0.9800
C48-H48A	0.9800	C65-H65C	0.9800
C48-H48B	0.9800	C66-H66A	0.9800
C48-H48C	0.9800	C66-H66B	0.9800
C49-H49A	0.9800	C66-H66C	0.9800
C49-H49B	0.9800	C67-C68	1.388(3)
C49-H49C	0.9800	C67-C72	1.392(3)
C50-H50A	0.9800	C67-H67	0.9500
C50-H50B	0.9800	C68-C69	1.378(4)
C50-H50C	0.9800	C68-H68	0.9500
C51-C52	1.550(3)	C69-C70	1.371(4)
C51-H51A	0.9800	C69-H69	0.9500
C51-H51B	0.9800	C70-C71	1.380(3)
C51-H51C	0.9800	C70-H70	0.9500
C52-C53	1.537(3)	C71-C72	1.406(3)
C52-C54	1.542(3)	C71-H71	0.9500
C53-H53A	0.9800	O1_2-C4_2	1.391(4)
C53-H53B	0.9800	O1_2-C1_2	1.412(4)
C53-H53C	0.9800	C1_2-C2_2	1.447(5)
C54-H54A	0.9800	C1_2-H1A_2	0.9900
C54-H54B	0.9800	C1_2-H1B_2	0.9900
C54-H54C	0.9800	C2_2-C3_2	1.507(5)
C55-C56	1.534(3)	C2_2-H2A_2	0.9900
C55-C57	1.545(3)	C2_2-H2B_2	0.9900
C55-C58	1.550(3)	C3_2-C4_2	1.478(5)
C56-H56A	0.9800	C3_2-H3A_2	0.9900
C56-H56B	0.9800	C3_2-H3B_2	0.9900
C56-H56C	0.9800	C4_2-H4A_2	0.9900
C57-H57A	0.9800	C4_2-H4B_2	0.9900
C57-H57B	0.9800	O1_3-C4_3	1.394(5)
C57-H57C	0.9800	O1_3-C1_3	1.450(5)
C58-H58A	0.9800	C1_3-C2_3	1.415(6)
C58-H58B	0.9800	C1_3-H1A_3	0.9900
C58-H58C	0.9800	C1_3-H1B_3	0.9900
C59-C61	1.540(4)	C2_3-C3_3	1.501(6)
C59-C62	1.542(4)	C2_3-H2A_3	0.9900
C59-C60	1.544(3)	C2_3-H2B_3	0.9900
C60-H60A	0.9800	C3_3-C4_3	1.474(5)
C60-H60B	0.9800	C3_3-H3A_3	0.9900
C60-H60C	0.9800	C3_3-H3B_3	0.9900

C4_3–H4A_3 0.9900
C4_3–H4B_3 0.9900

Atom–Atom–Atom Angle [°]

P5–Cu1–P4 129.66(3)
P5–Cu1–P1 130.14(4)
P4–Cu1–P1 98.75(4)
C19–P1–C25 103.60(9)
C19–P1–Cu2 106.58(7)
C25–P1–Cu2 102.99(7)
C19–P1–Cu1 109.42(8)
C25–P1–Cu1 117.51(6)
Cu2–P1–Cu1 115.59(4)
P2–Cu2–P1 167.32(3)
P2–Cu2–Cu4 96.16(2)
P1–Cu2–Cu4 95.68(3)
C37–P2–C31 102.48(10)
C37–P2–Cu2 111.13(8)
C31–P2–Cu2 101.77(7)
C37–P2–Cu3 110.63(7)
C31–P2–Cu3 117.44(8)
Cu2–P2–Cu3 112.70(3)
P6–Cu3–P2 132.84(3)
P6–Cu3–P3 127.65(3)
P2–Cu3–P3 98.62(4)
C72–P3–C1 100.15(10)
C72–P3–Cu4 109.04(8)
C1–P3–Cu4 105.18(7)
C72–P3–Cu3 125.56(7)
C1–P3–Cu3 114.54(7)
Cu4–P3–Cu3 100.98(4)
P3–Cu4–P4 173.43(2)
P3–Cu4–Cu2 92.32(3)
P4–Cu4–Cu2 94.02(3)
C7–P4–C13 100.35(10)
C7–P4–Cu4 106.18(8)
C13–P4–Cu4 104.14(7)
C7–P4–Cu1 125.93(7)
C13–P4–Cu1 113.23(8)
Cu4–P4–Cu1 105.06(4)
C55–P5–C59 109.61(12)
C55–P5–C63 108.56(12)
C59–P5–C63 108.43(11)
C55–P5–Cu1 105.07(8)
C59–P5–Cu1 109.29(8)
C63–P5–Cu1 115.75(8)
C47–P6–C52 109.11(10)
C47–P6–C43 108.12(10)
C52–P6–C43 107.94(11)
C47–P6–Cu3 107.97(8)
C52–P6–Cu3 107.83(7)
C43–P6–Cu3 115.73(7)
C2–C1–C6 117.5(2)

C2–C1–P3 121.90(18)
C6–C1–P3 120.65(18)
C1–C2–C3 121.2(3)
C1–C2–H2 119.4
C3–C2–H2 119.4
C4–C3–C2 120.4(3)
C4–C3–H3 119.8
C2–C3–H3 119.8
C3–C4–C5 119.7(3)
C3–C4–H4 120.1
C5–C4–H4 120.1
C4–C5–C6 119.7(3)
C4–C5–H5 120.2
C6–C5–H5 120.2
C5–C6–C1 121.4(3)
C5–C6–H6 119.3
C1–C6–H6 119.3
C12–C7–C8 117.3(2)
C12–C7–P4 122.22(17)
C8–C7–P4 120.45(17)
C9–C8–C7 121.6(2)
C9–C8–H8 119.2
C7–C8–H8 119.2
C10–C9–C8 120.1(2)
C10–C9–H9 119.9
C8–C9–H9 119.9
C9–C10–C11 119.6(2)
C9–C10–H10 120.2
C11–C10–H10 120.2
C10–C11–C12 120.2(2)
C10–C11–H11 119.9
C12–C11–H11 119.9
C11–C12–C7 121.1(2)
C11–C12–H12 119.5
C7–C12–H12 119.5
C14–C13–C18 117.4(2)
C14–C13–P4 122.04(16)
C18–C13–P4 120.57(16)
C13–C14–C15 121.0(2)
C13–C14–H14 119.5
C15–C14–H14 119.5
C16–C15–C14 120.4(2)
C16–C15–H15 119.8
C14–C15–H15 119.8
C17–C16–C15 119.5(2)
C17–C16–H16 120.2
C15–C16–H16 120.2
C16–C17–C18 120.4(2)
C16–C17–H17 119.8
C18–C17–H17 119.8
C17–C18–C13 121.2(2)
C17–C18–H18 119.4
C13–C18–H18 119.4

C24-C19-C20	117.4(2)	C31-C36-H36	119.4
C24-C19-P1	121.32(16)	C42-C37-C38	117.1(2)
C20-C19-P1	121.13(17)	C42-C37-P2	120.37(17)
C19-C20-C21	121.1(2)	C38-C37-P2	122.47(18)
C19-C20-H20	119.4	C39-C38-C37	121.0(2)
C21-C20-H20	119.4	C39-C38-H38	119.5
C22-C21-C20	120.4(2)	C37-C38-H38	119.5
C22-C21-H21	119.8	C40-C39-C38	120.3(3)
C20-C21-H21	119.8	C40-C39-H39	119.8
C23-C22-C21	119.6(2)	C38-C39-H39	119.8
C23-C22-H22	120.2	C39-C40-C41	120.2(3)
C21-C22-H22	120.2	C39-C40-H40	119.9
C19-C24-C23	121.7(2)	C41-C40-H40	119.9
C19-C24-H24	119.2	C40-C41-C42	119.7(3)
C23-C24-H24	119.2	C40-C41-H41	120.2
C22-C23-C24	119.8(2)	C42-C41-H41	120.2
C22-C23-H23	120.1	C37-C42-C41	121.7(2)
C24-C23-H23	120.1	C37-C42-H42	119.2
C26-C25-C30	117.8(2)	C41-C42-H42	119.2
C26-C25-P1	124.05(17)	C44-C43-C45	105.1(2)
C30-C25-P1	118.09(17)	C44-C43-C46	108.48(19)
C25-C26-C27	121.5(2)	C45-C43-C46	108.77(19)
C25-C26-H26	119.3	C44-C43-P6	109.22(16)
C27-C26-H26	119.3	C45-C43-P6	108.93(15)
C28-C27-C26	120.3(2)	C46-C43-P6	115.77(16)
C28-C27-H27	119.9	C43-C44-H44A	109.5
C26-C27-H27	119.9	C43-C44-H44B	109.5
C27-C28-C29	118.8(2)	H44A-C44-H44B	109.5
C27-C28-H28	120.6	C43-C44-H44C	109.5
C29-C28-H28	120.6	H44A-C44-H44C	109.5
C30-C29-C28	120.8(2)	H44B-C44-H44C	109.5
C30-C29-H29	119.6	C43-C45-H45A	109.5
C28-C29-H29	119.6	C43-C45-H45B	109.5
C29-C30-C25	120.9(2)	H45A-C45-H45B	109.5
C29-C30-H30	119.6	C43-C45-H45C	109.5
C25-C30-H30	119.6	H45A-C45-H45C	109.5
C32-C31-C36	117.7(2)	H45B-C45-H45C	109.5
C32-C31-P2	124.26(17)	C43-C46-H46A	109.5
C36-C31-P2	117.99(17)	C43-C46-H46B	109.5
C31-C32-C33	121.1(2)	H46A-C46-H46B	109.5
C31-C32-H32	119.4	C43-C46-H46C	109.5
C33-C32-H32	119.4	H46A-C46-H46C	109.5
C34-C33-C32	119.9(3)	H46B-C46-H46C	109.5
C34-C33-H33	120.1	C50-C47-C48	105.5(2)
C32-C33-H33	120.1	C50-C47-C49	109.0(2)
C35-C34-C33	120.1(2)	C48-C47-C49	108.10(19)
C35-C34-H34	119.9	C50-C47-P6	108.19(15)
C33-C34-H34	119.9	C48-C47-P6	109.43(16)
C34-C35-C36	120.0(2)	C49-C47-P6	116.11(17)
C34-C35-H35	120.0	C47-C48-H48A	109.5
C36-C35-H35	120.0	C47-C48-H48B	109.5
C35-C36-C31	121.1(2)	H48A-C48-H48B	109.5
C35-C36-H36	119.4	C47-C48-H48C	109.5

H48A-C48-H48C	109.5	C55-C57-H57C	109.5
H48B-C48-H48C	109.5	H57A-C57-H57C	109.5
C47-C49-H49A	109.5	H57B-C57-H57C	109.5
C47-C49-H49B	109.5	C55-C58-H58A	109.5
H49A-C49-H49B	109.5	C55-C58-H58B	109.5
C47-C49-H49C	109.5	H58A-C58-H58B	109.5
H49A-C49-H49C	109.5	C55-C58-H58C	109.5
H49B-C49-H49C	109.5	H58A-C58-H58C	109.5
C47-C50-H50A	109.5	H58B-C58-H58C	109.5
C47-C50-H50B	109.5	C61-C59-C62	105.4(2)
H50A-C50-H50B	109.5	C61-C59-C60	108.6(2)
C47-C50-H50C	109.5	C62-C59-C60	108.9(2)
H50A-C50-H50C	109.5	C61-C59-P5	108.48(17)
H50B-C50-H50C	109.5	C62-C59-P5	108.63(17)
C52-C51-H51A	109.5	C60-C59-P5	116.25(17)
C52-C51-H51B	109.5	C59-C60-H60A	109.5
H51A-C51-H51B	109.5	C59-C60-H60B	109.5
C52-C51-H51C	109.5	H60A-C60-H60B	109.5
H51A-C51-H51C	109.5	C59-C60-H60C	109.5
H51B-C51-H51C	109.5	H60A-C60-H60C	109.5
C53-C52-C54	107.81(19)	H60B-C60-H60C	109.5
C53-C52-C51	104.51(18)	C59-C61-H61A	109.5
C54-C52-C51	110.39(19)	C59-C61-H61B	109.5
C53-C52-P6	109.86(15)	H61A-C61-H61B	109.5
C54-C52-P6	116.81(16)	C59-C61-H61C	109.5
C51-C52-P6	106.77(15)	H61A-C61-H61C	109.5
C52-C53-H53A	109.5	H61B-C61-H61C	109.5
C52-C53-H53B	109.5	C59-C62-H62A	109.5
H53A-C53-H53B	109.5	C59-C62-H62B	109.5
C52-C53-H53C	109.5	H62A-C62-H62B	109.5
H53A-C53-H53C	109.5	C59-C62-H62C	109.5
H53B-C53-H53C	109.5	H62A-C62-H62C	109.5
C52-C54-H54A	109.5	H62B-C62-H62C	109.5
C52-C54-H54B	109.5	C66-C63-C64	106.2(2)
H54A-C54-H54B	109.5	C66-C63-C65	109.1(2)
C52-C54-H54C	109.5	C64-C63-C65	107.4(2)
H54A-C54-H54C	109.5	C66-C63-P5	108.87(19)
H54B-C54-H54C	109.5	C64-C63-P5	109.14(16)
C56-C55-C57	108.1(2)	C65-C63-P5	115.61(18)
C56-C55-C58	105.3(2)	C63-C64-H64A	109.5
C57-C55-C58	110.0(2)	C63-C64-H64B	109.5
C56-C55-P5	110.58(17)	H64A-C64-H64B	109.5
C57-C55-P5	116.17(18)	C63-C64-H64C	109.5
C58-C55-P5	106.16(16)	H64A-C64-H64C	109.5
C55-C56-H56A	109.5	H64B-C64-H64C	109.5
C55-C56-H56B	109.5	C63-C65-H65A	109.5
H56A-C56-H56B	109.5	C63-C65-H65B	109.5
C55-C56-H56C	109.5	H65A-C65-H65B	109.5
H56A-C56-H56C	109.5	C63-C65-H65C	109.5
H56B-C56-H56C	109.5	H65A-C65-H65C	109.5
C55-C57-H57A	109.5	H65B-C65-H65C	109.5
C55-C57-H57B	109.5	C63-C66-H66A	109.5
H57A-C57-H57B	109.5	C63-C66-H66B	109.5

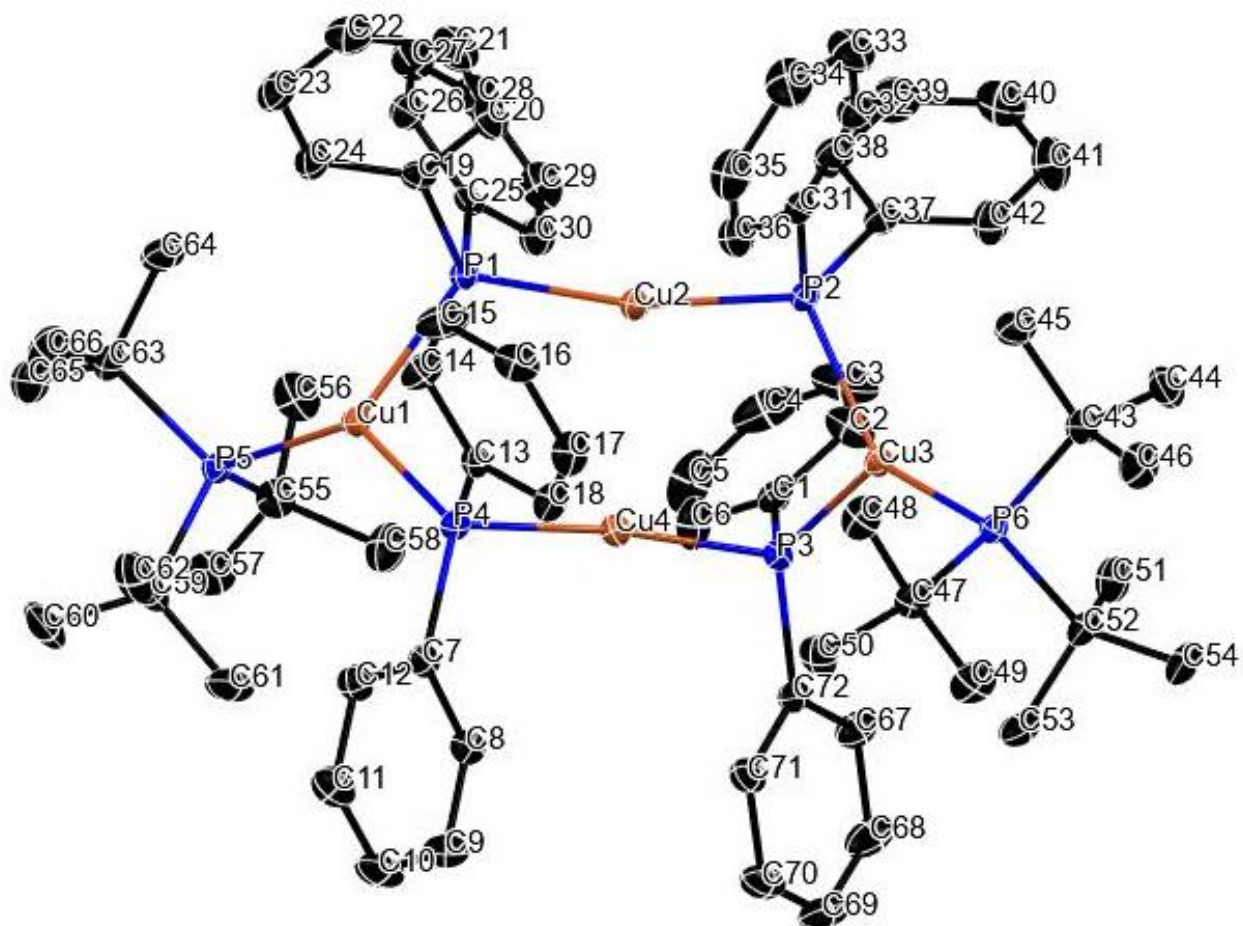
H66A–C66–H66B	109.5
C63–C66–H66C	109.5
H66A–C66–H66C	109.5
H66B–C66–H66C	109.5
C68–C67–C72	120.8(3)
C68–C67–H67	119.6
C72–C67–H67	119.6
C69–C68–C67	120.9(3)
C69–C68–H68	119.5
C67–C68–H68	119.5
C70–C69–C68	119.2(2)
C70–C69–H69	120.4
C68–C69–H69	120.4
C69–C70–C71	120.6(3)
C69–C70–H70	119.7
C71–C70–H70	119.7
C70–C71–C72	121.3(2)
C70–C71–H71	119.4
C72–C71–H71	119.4
C67–C72–C71	117.2(2)
C67–C72–P3	121.96(18)
C71–C72–P3	120.75(17)
C4_2–O1_2–C1_2	107.8(3)
O1_2–C1_2–C2_2	105.9(3)
O1_2–C1_2–H1A_2	110.6
C2_2–C1_2–H1A_2	110.6
O1_2–C1_2–H1B_2	110.6
C2_2–C1_2–H1B_2	110.6
H1A_2–C1_2–H1B_2	108.7
C1_2–C2_2–C3_2	102.0(3)
C1_2–C2_2–H2A_2	111.4
C3_2–C2_2–H2A_2	111.4
C1_2–C2_2–H2B_2	111.4
C3_2–C2_2–H2B_2	111.4
H2A_2–C2_2–H2B_2	109.2
C4_2–C3_2–C2_2	101.3(3)
C4_2–C3_2–H3A_2	111.5
C2_2–C3_2–H3A_2	111.5
C4_2–C3_2–H3B_2	111.5
C2_2–C3_2–H3B_2	111.5
H3A_2–C3_2–H3B_2	109.3
O1_2–C4_2–C3_2	108.7(3)
O1_2–C4_2–H4A_2	110.0
C3_2–C4_2–H4A_2	110.0
O1_2–C4_2–H4B_2	110.0
C3_2–C4_2–H4B_2	110.0
H4A_2–C4_2–H4B_2	108.3
C4_3–O1_3–C1_3	108.7(3)
C2_3–C1_3–O1_3	107.5(4)
C2_3–C1_3–H1A_3	110.2
O1_3–C1_3–H1A_3	110.2
C2_3–C1_3–H1B_3	110.2
O1_3–C1_3–H1B_3	110.2

H1A_3–C1_3–H1B_3	108.5
C1_3–C2_3–C3_3	104.2(4)
C1_3–C2_3–H2A_3	110.9
C3_3–C2_3–H2A_3	110.9
C1_3–C2_3–H2B_3	110.9
C3_3–C2_3–H2B_3	110.9
H2A_3–C2_3–H2B_3	108.9
C4_3–C3_3–C2_3	103.5(3)
C4_3–C3_3–H3A_3	111.1
C2_3–C3_3–H3A_3	111.1
C4_3–C3_3–H3B_3	111.1
C2_3–C3_3–H3B_3	111.1
H3A_3–C3_3–H3B_3	109.0
O1_3–C4_3–C3_3	107.1(4)
O1_3–C4_3–H4A_3	110.3
C3_3–C4_3–H4A_3	110.3
O1_3–C4_3–H4B_3	110.3
C3_3–C4_3–H4B_3	110.3
H4A_3–C4_3–H4B_3	108.5

Atom–Atom–Atom–Atom	Torsion Angle [°]
C72–P3–C1–C2	–116.3(2)
Cu4–P3–C1–C2	130.63(19)
Cu3–P3–C1–C2	20.7(2)
C72–P3–C1–C6	63.3(2)
Cu4–P3–C1–C6	–49.8(2)
Cu3–P3–C1–C6	–159.74(17)
C6–C1–C2–C3	1.9(4)
P3–C1–C2–C3	–178.5(2)
C1–C2–C3–C4	–2.1(4)
C2–C3–C4–C5	0.1(5)
C3–C4–C5–C6	2.0(5)
C4–C5–C6–C1	–2.1(4)
C2–C1–C6–C5	0.2(4)
P3–C1–C6–C5	–179.4(2)
C13–P4–C7–C12	43.63(19)
Cu4–P4–C7–C12	151.78(16)
Cu1–P4–C7–C12	–85.23(19)
C13–P4–C7–C8	–137.51(18)
Cu4–P4–C7–C8	–29.36(19)
Cu1–P4–C7–C8	93.63(18)
C12–C7–C8–C9	–1.8(3)
P4–C7–C8–C9	179.34(18)
C7–C8–C9–C10	0.9(4)
C8–C9–C10–C11	0.6(4)
C9–C10–C11–C12	–1.3(4)
C10–C11–C12–C7	0.5(4)
C8–C7–C12–C11	1.0(3)
P4–C7–C12–C11	179.94(18)
C7–P4–C13–C14	–126.20(19)
Cu4–P4–C13–C14	124.04(18)
Cu1–P4–C13–C14	10.5(2)

C7-P4-C13-C18	55.87(19)	P2-C31-C36-C35	178.24(19)
Cu4-P4-C13-C18	-53.89(18)	C31-P2-C37-C42	85.1(2)
Cu1-P4-C13-C18	-167.45(15)	Cu2-P2-C37-C42	-166.84(17)
C18-C13-C14-C15	1.1(3)	Cu3-P2-C37-C42	-40.9(2)
P4-C13-C14-C15	-176.87(19)	C31-P2-C37-C38	-96.3(2)
C13-C14-C15-C16	-0.7(4)	Cu2-P2-C37-C38	11.7(2)
C14-C15-C16-C17	-0.6(4)	Cu3-P2-C37-C38	137.69(18)
C15-C16-C17-C18	1.5(4)	C42-C37-C38-C39	-1.4(4)
C16-C17-C18-C13	-1.1(4)	P2-C37-C38-C39	-180.0(2)
C14-C13-C18-C17	-0.2(3)	C37-C38-C39-C40	0.4(4)
P4-C13-C18-C17	177.81(18)	C38-C39-C40-C41	0.5(5)
C25-P1-C19-C24	89.81(19)	C39-C40-C41-C42	-0.3(5)
Cu2-P1-C19-C24	-161.93(17)	C38-C37-C42-C41	1.6(4)
Cu1-P1-C19-C24	-36.3(2)	P2-C37-C42-C41	-179.8(2)
C25-P1-C19-C20	-95.08(19)	C40-C41-C42-C37	-0.8(4)
Cu2-P1-C19-C20	13.18(19)	C72-C67-C68-C69	-0.6(4)
Cu1-P1-C19-C20	138.83(17)	C67-C68-C69-C70	0.1(4)
C24-C19-C20-C21	-0.4(4)	C68-C69-C70-C71	0.2(4)
P1-C19-C20-C21	-175.7(2)	C69-C70-C71-C72	0.1(4)
C19-C20-C21-C22	0.3(4)	C68-C67-C72-C71	0.8(3)
C20-C21-C22-C23	0.1(4)	C68-C67-C72-P3	177.95(18)
C20-C19-C24-C23	0.2(4)	C70-C71-C72-C67	-0.6(3)
P1-C19-C24-C23	175.48(19)	C70-C71-C72-P3	-177.78(17)
C21-C22-C23-C24	-0.3(4)	C1-P3-C72-C67	36.9(2)
C19-C24-C23-C22	0.2(4)	Cu4-P3-C72-C67	146.96(17)
C19-P1-C25-C26	-25.8(2)	Cu3-P3-C72-C67	-93.40(19)
Cu2-P1-C25-C26	-136.69(17)	C1-P3-C72-C71	-146.10(18)
Cu1-P1-C25-C26	95.00(18)	Cu4-P3-C72-C71	-36.03(19)
C19-P1-C25-C30	155.50(17)	Cu3-P3-C72-C71	83.60(19)
Cu2-P1-C25-C30	44.58(17)	C4_2-O1_2-C1_2-C2_2	24.8(4)
Cu1-P1-C25-C30	-83.74(18)	O1_2-C1_2-C2_2-C3_2	-37.1(4)
C30-C25-C26-C27	0.6(3)	C1_2-C2_2-C3_2-C4_2	34.6(4)
P1-C25-C26-C27	-178.13(18)	C1_2-O1_2-C4_2-C3_2	-1.5(5)
C25-C26-C27-C28	-0.1(4)	C2_2-C3_2-C4_2-O1_2	-20.9(5)
C26-C27-C28-C29	-0.3(4)	C4_3-O1_3-C1_3-C2_3	11.2(6)
C27-C28-C29-C30	0.0(4)	O1_3-C1_3-C2_3-C3_3	-25.5(5)
C28-C29-C30-C25	0.6(4)	C1_3-C2_3-C3_3-C4_3	30.0(5)
C26-C25-C30-C29	-0.8(3)	C1_3-O1_3-C4_3-C3_3	8.5(5)
P1-C25-C30-C29	177.97(19)	C2_3-C3_3-C4_3-O1_3	-23.6(5)
C37-P2-C31-C32	-7.3(2)		
Cu2-P2-C31-C32	-122.31(19)		
Cu3-P2-C31-C32	114.17(19)		
C37-P2-C31-C36	172.90(17)		
Cu2-P2-C31-C36	57.86(18)		
Cu3-P2-C31-C36	-65.67(18)		
C36-C31-C32-C33	1.7(4)		
P2-C31-C32-C33	-178.1(2)		
C31-C32-C33-C34	-0.3(4)		
C32-C33-C34-C35	-1.3(5)		
C33-C34-C35-C36	1.5(4)		
C34-C35-C36-C31	0.0(4)		
C32-C31-C36-C35	-1.6(3)		

Figure S14



Molecular structure of **1** with thermal ellipsoids drawn at the 30% probability level. Hydrogen atoms and two non-coordinated THF molecules of solvation are omitted for clarity.