Supplementary information

Ultrafast electronic, infrared, and X-ray absorption spectroscopic study of Cu(I) phosphine diimine complexes

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1. Synthesis

4,4'-di(COOEt)-2,2'-biquinoline (deebq)

The ligand was synthesised following literature procedure given in brief here.[1] 4,4'-dicarboxylic-acid-2,2'-biquinoline (0.5 g, 1.45 mmol) was added to ethanol (23 ml) and was chilled in an ice bath to ~0 C˚. Sulfuric acid (34.6 ml, 17.85 M) was added dropwise to the suspension which fully dissolved after 1 hour to give a cream-coloured solution. The solution was then refluxed for 27 h at 80 C˚. Following reflux, the solution was neutralised with NaOH (133 ml, 25% w/v, 7.81 M) producing a white precipitate. The resulting precipitate was filtered to yield a white powder (349.6 mg, 64% yield).

4,4'-di(COOEt) 2,2'-biquinoline: ^{1}H NMR (400 MHz, $CDCl_3$): 9.33 (2H, s), 8.82 (2H, d, J= 8.4 Hz), 8.36 (2H, d, J= 8.4 Hz), 7.90-7.80 (2H, m), 7.73 (2H, m, J= 8.3, 6.9, 1.2 Hz), 4.63 (4H, q, J= 7.1 Hz), 1.58 (6H, t, J= 8.0 Hz). m/z (ES+) 401.2 (100%, M+)

$[Cu(deebq)_2]BF_4$ (D1)

deebq (107 mg, 0.42 mmol) and $[Cu(CH_3CN)_4](BF_4)$ (52 mg, 0.16 mmol) were dissolved in dry DCM (10 mL) under N_2. The solution was then stirred for 1 h. The solvent was reduced to minimal volume (~2 mL) by rotary evaporation. A dark blue precipitate crashed out of solution upon addition of diethyl ether. The product was dried in a vacuum desiccator, yielding a dark-blue powder (122 mg, 93%).

$[Cu(deebq)_2]$BF4: ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 9.38 (4H, s), 8.86 (4H, d, J=8.0 Hz), 7.73 (4H, d, J=8.5 Hz), 7.68 (4H, t, J=7.5 Hz), 7.45 (4H, t, J=7.5 Hz), 4.76 (8H, q, J=7.4 Hz), 1.58 (12H, t, J=7.1 Hz). m/z (ES+) 863.4 (100%, M^+)

[Cu(xantphos)(deebq)]BF_4 (D2)

Complexes D2 and D3 were synthesised following an adapted literature procedure.[2] xantphos (166 mg, 0.29 mmol) and $[Cu(CH_3CN)_4](BF_4)$ (100 mg, 0.33 mmol) were dissolved in dry DCM (10 mL). The solution was then stirred for 1 h. While the solution was stirred, deebq (108 mg, 0.42 mmol) dissolved in DCM (5mL) was added. The solution was stirred for a further hour. The solvent was reduced to minimal volume (~2 mL) by rotary evaporation. A dark orange precipitate crashed out of solution upon addition of diethyl ether. The product was dried in a vacuum desiccator to yield a dark-orange powder. (244 mg, 76%).

[Cu(xantphos)(deebq)]BF4: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (2H, s, dcbq), 8.76 (2H, d, J=7.8 Hz, dcbq), 7.98 (2H, d, J=8.2 Hz, dcbq), 7.78 (2H, d, J=8.2 Hz), 7.64 (2H, t, J=7.8 Hz), 7.35-7.29 (4H, m), 7.26-7.02 (10H, m, xantphos), 6.94-6.89 (2H, m), 4.71 (4H, q, J=7.1 Hz, dcbq), 1.94 (6H, s, xantphos), 1.55 (6H, t, J= 7.1 Hz, dcbq). m/z (ES+) 1041.3 (100%, M^+)

[Cu(DPEphos)(deebq)]BF_4 (D3)

DPEphos (150 mg, 0.28 mmol) and [Cu($CH_3CN)_4$](BF_4) (100 mg, 0.33 mmol) were dissolved in dry DCM (10 mL).The solution was then stirred for 1 h. While the solution was stirred, dcbq (106 mg, 0.41 mmol) dissolved in DCM (5mL) was added. The solution was stirred for a further hour. The solvent was reduced to minimal volume (~2 mL) by rotary evaporation. A dark orange precipitate crashed out of solution upon addition of diethyl ether. The product was dried in a vacuum desiccator, yielding a dark-orange powder (141 mg, 46%).

[Cu(DPEphos)(deebq)]BF4: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (2H, d, J=8.2 Hz, DPEphos), 8.71 (2H, s, dcbq), 8.44 (2H, d, J= 8.2 Hz, dcbq), 7.69-7.63 (2H, m, dcbq), 7.50-7.40 (2H, m), 7.25-7.12 (10H, m), 6.92 (8H, dd, J=29.1, 21.8 Hz, DPEphos), 6.71 (8H, dd, J=29.1, 21.8 Hz, DPEphos), 4.70 (4H, q, J= 7.1 Hz, dcbq), 1.53 (6H, t, J=8.0 Hz, dcbq). m/z (ES+) 1001.3 (100%, M^+)

2. Steady-state electronic spectroscopy

Table S1. Absorption band maxima (λ_{max}/nm) for **D1-D3** in different solvents

Solvent	Dielelectric constant[a]	Dipole moment[a]	Viscosity 10^{-3} Pa s[a]	**D1**	**D2**	**D3**
Hexane	1.9	0.1	0.29	581	-	-
Chloroform	4.8	1.0	0.54	581	496	496
DCM	8.9	1.6	0.42	579	499	496
Acetone	21	2.85	0.30	577	489	483
Ethanol	24	1.7	1.08	581	490	496

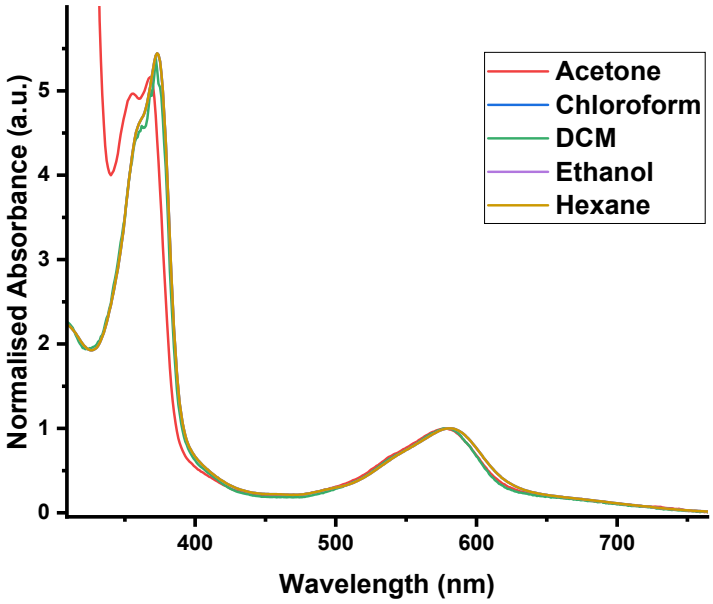

Figure S1. Normalised UV-vis absorption of [Cu($deebq)_2$]BF_4 (**D1**) in acetone (red), chloroform (blue), DCM (green), ethanol (purple) and Hexane (yellow). The spectra are normalised to the absorption maximum of the MLCT band.

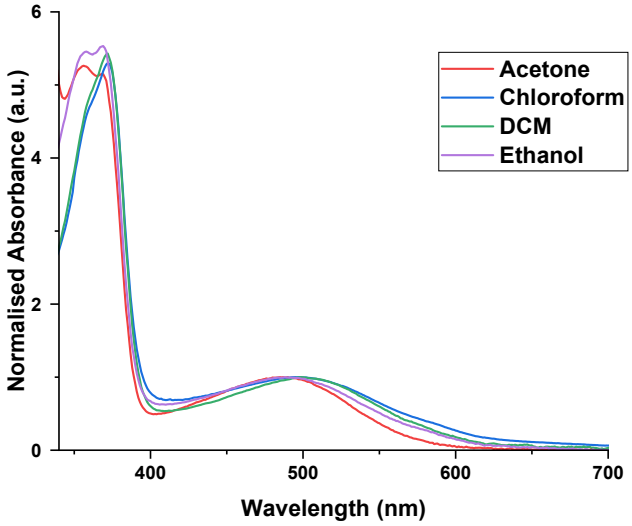

Figure S2. Normalised UV-vis absorption of [Cu(xantphos)(deebq)]BF_4 (**D2**) in acetone (red), chloroform (blue), DCM (green) and ethanol (purple). The spectra are normalised to the absorption maximum of the MLCT band. The second absorption band at ~575 nm is tentatively assigned to formation of **D1** via ligand scrambling.

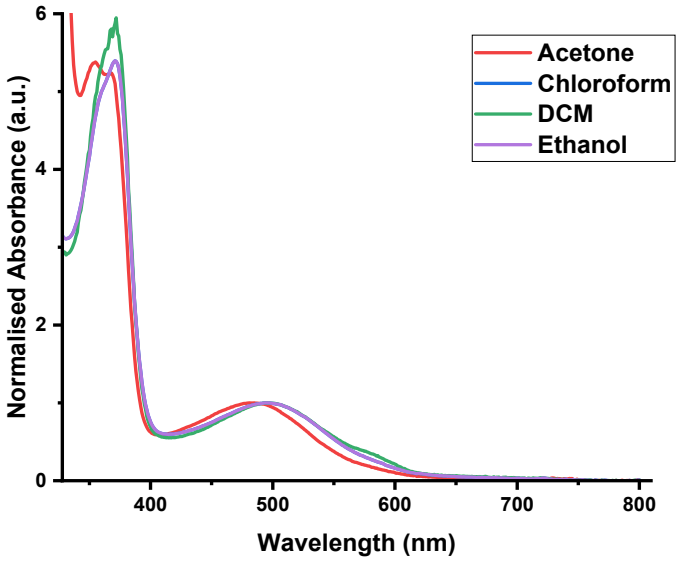

Figure S3. Normalised UV-vis absorption of [Cu(DPEphos)(deebq)]BF_4 (**D3**) in acetone (red), chloroform (blue), DCM (green) and ethanol (purple). The spectra are normalised to the absorption maximum of the MLCT band. The second absorption band at ~575 nm is tentatively assigned to formation of **D1** via ligand scrambling.

3. Transient absorption spectroscopy

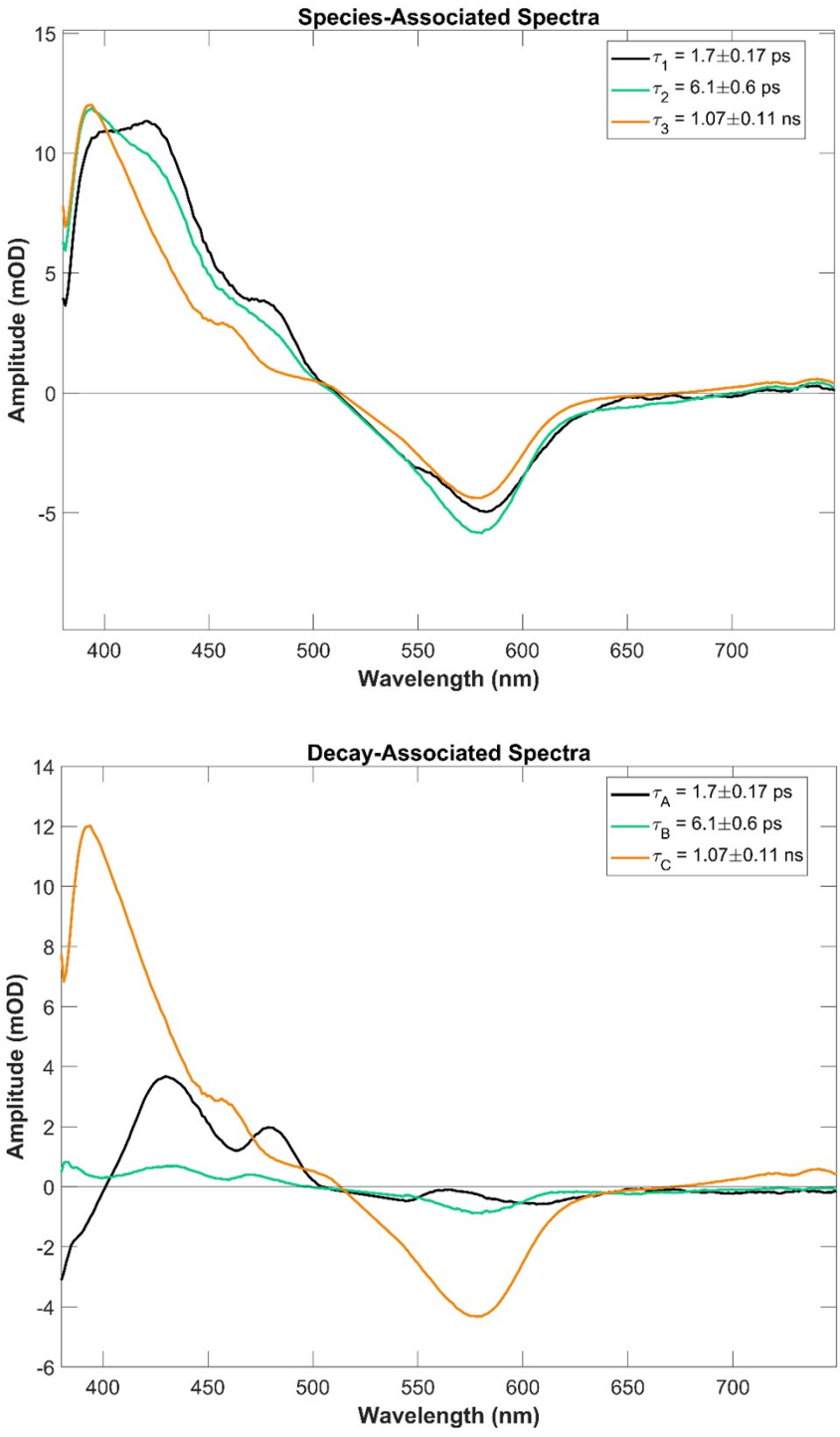

Figure S4. Top: Species-Associated Spectra (SAS) and, Bottom: Decay-Associated Spectra (DAS) for the fs-transient absorption spectra of $[Cu(deebq)_2]BF_4$ (**D1**) in DCM, after photoexcitation from 525 nm (OD@525nm=0.2, 2 mW), collected with the pump set to magic angle (54.7 ˚) with respect to the probe. The time delay between the pump and probe for each spectrum is shown in the legend. The spectra have been cropped between 510 and 540 nm to remove pump scatter.

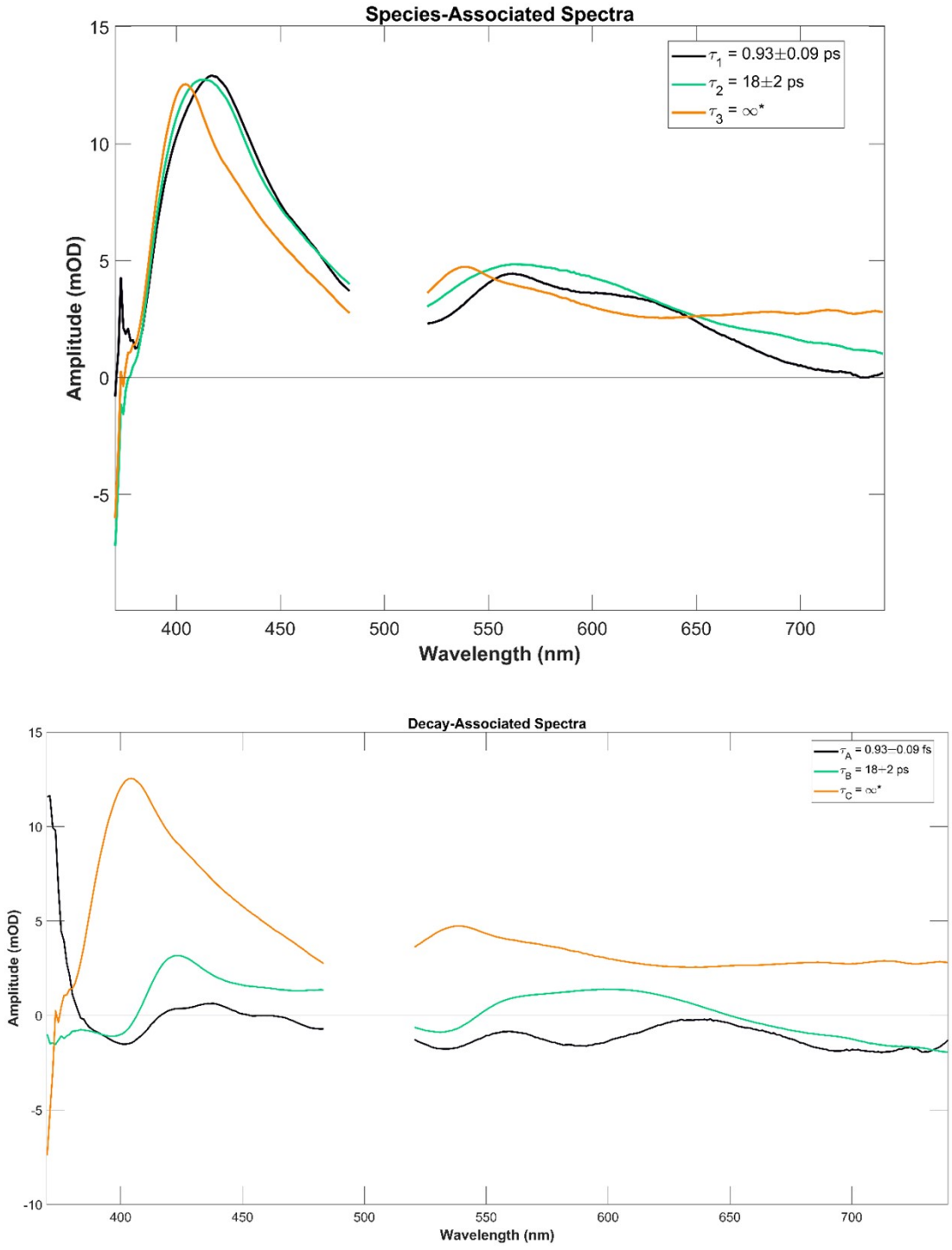

Figure S5. Top: Species-Associated Spectra (SAS) and, Bottom: Decay-Associated Spectra (DAS) for the fs-transient absorption spectra of [Cu(xant)(deebq)]BF_4 (**D2**) in DCM, after photoexcitation from 500 nm (OD@500nm=0.38, 2 mW), collected with the pump set to magic angle (54.7 ˚) with respect to the probe. The time delay between the pump and probe for each spectrum is shown in the legend. The spectra have been cropped between 510 and 540 nm to remove pump scatter.

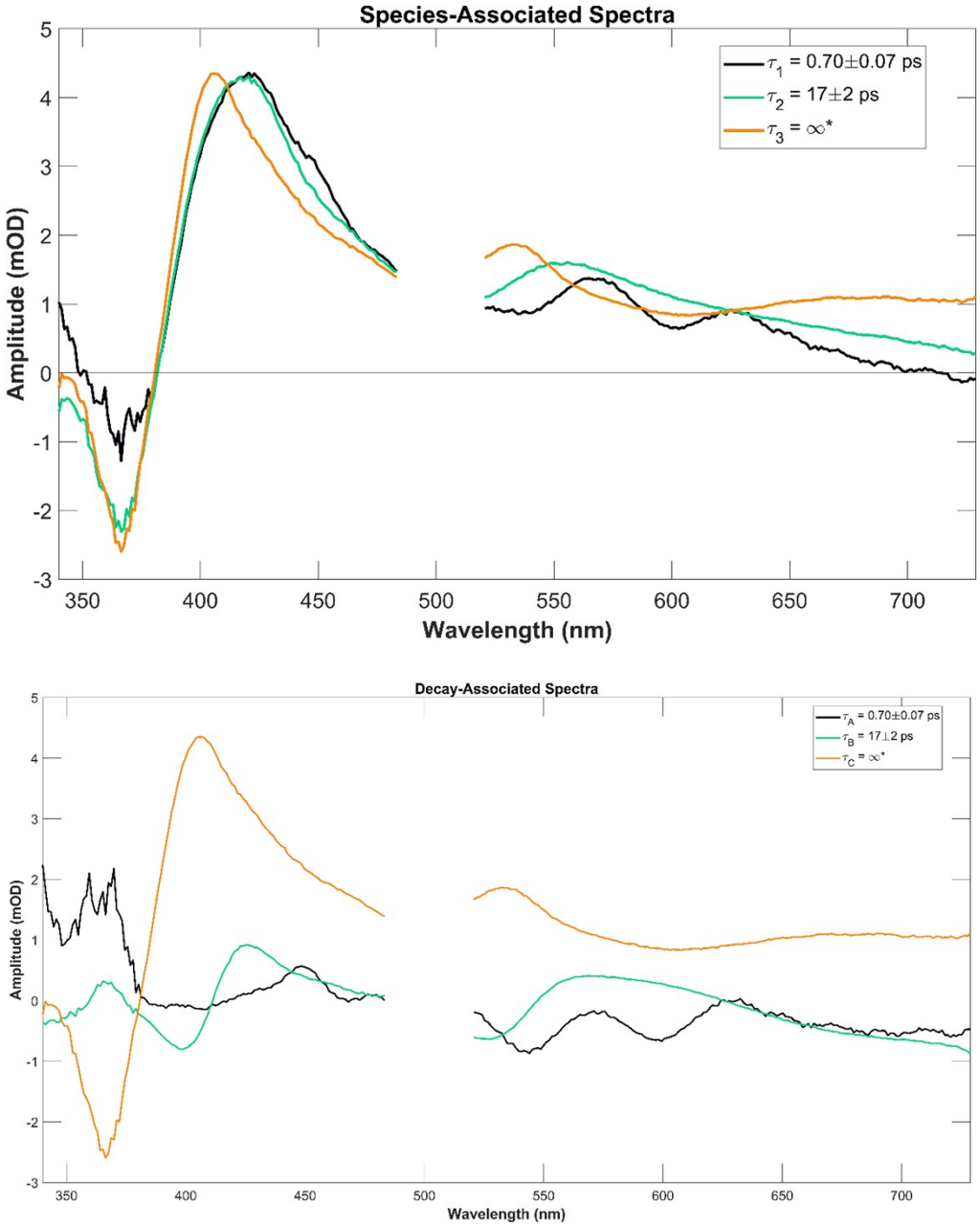

Figure S6. Top: Species-Associated Spectra (SAS) and, Bottom: Decay-Associated Spectra (DAS) for the fs-transient absorption spectra of [Cu(DPEphos)(deebq)]BF_4 (**D3**) in DCM, after photoexcitation from 500 nm (OD@500nm=0.2, 2 mW), collected with the pump set to magic angle (54.7 ˚) with respect to the probe. The time delay between the pump and probe for each spectrum is shown in the legend. The spectra have been cropped between 510 and 540 nm to remove pump scatt

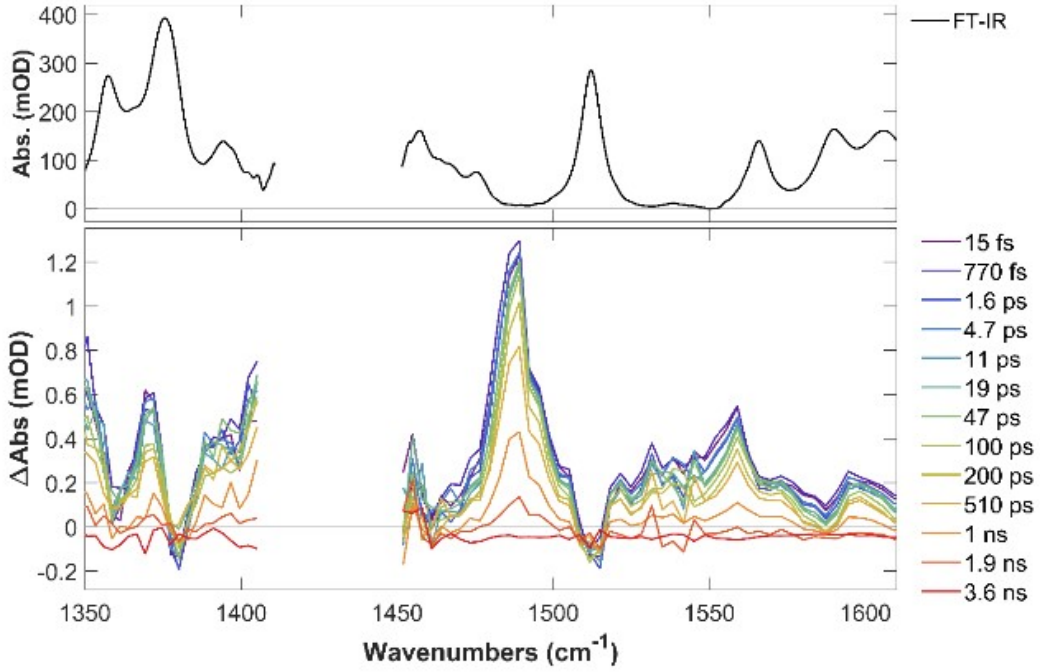

Figure S7. TRIR spectra of $[Cu(deebq)_2]BF_4$ (**D1**) from 1350-1625 cm^{-1} in DCM following excitation at 525 nm (2 mW, OD@525nm = 0.6), collected with the pump set to magic angle (54.7 ˚) with respect to the probe. The time delay between the pump and probe for each spectrum is shown in the legend.

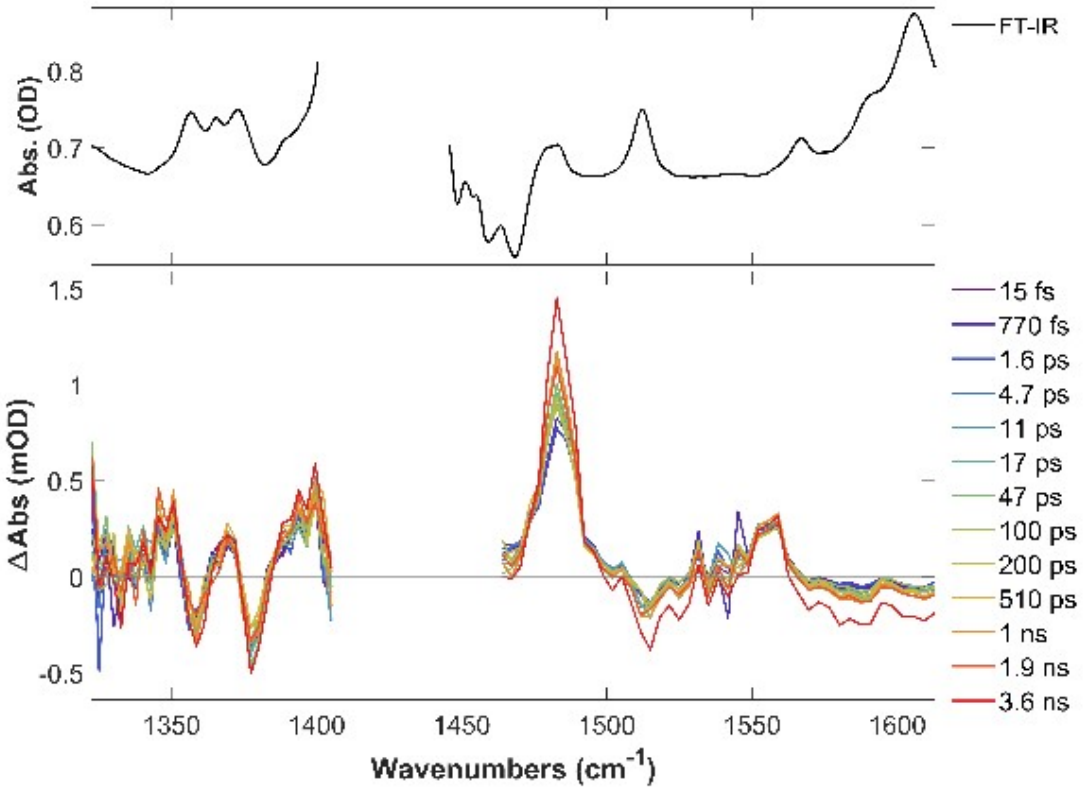

Figure S8. TRIR spectra of $[Cu(xant)(deebq)]BF_4$ (**D2**) from 1300-1650 cm^{-1}. TRIR spectra were recorded in DCM following excitation at 500 nm (2 mW, OD@500nm = 0.6), collected with the pump set to magic angle (54.7 ˚) with respect to the probe. The time delay between the pump and probe for each spectrum is shown in the legend.

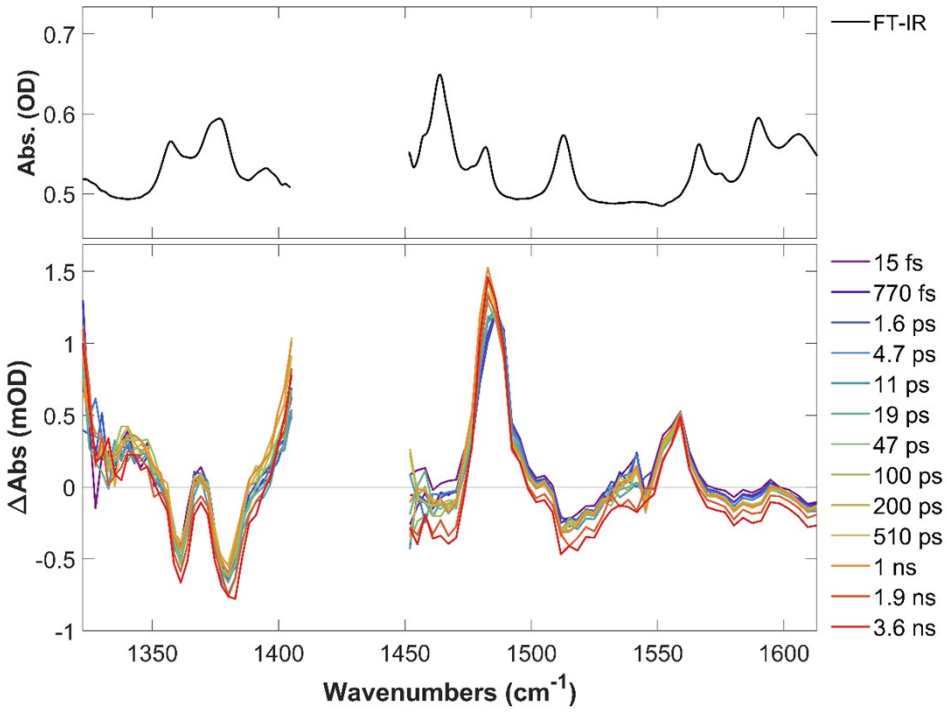

Figure S9. TRIR spectra of [Cu(DPEphos)(deebq)]BF4 (D3) from 1340-1620 cm^{-1}. TRIR spectra were recorded in DCM following excitation at 530 nm (2 mW, OD@530nm = 0.65), collected with the pump set to magic angle (54.7 ˚) with respect to the probe. The time delay between the pump and probe for each spectrum is shown in the legend.

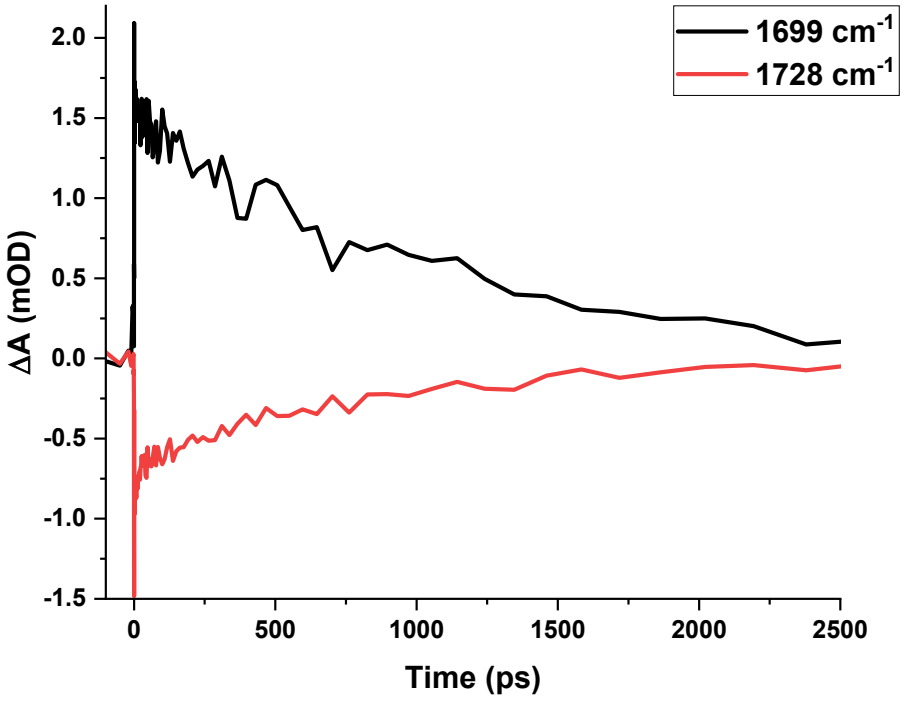

Figure S10. TRIR kinetics of $[Cu(deebq)_2]BF_4$ (**D1**) in DCM following excitation at 525 nm (2 mW, OD@525nm = 0.6), collected with the pump set to magic angle (54.7 ˚) with respect to the probe.

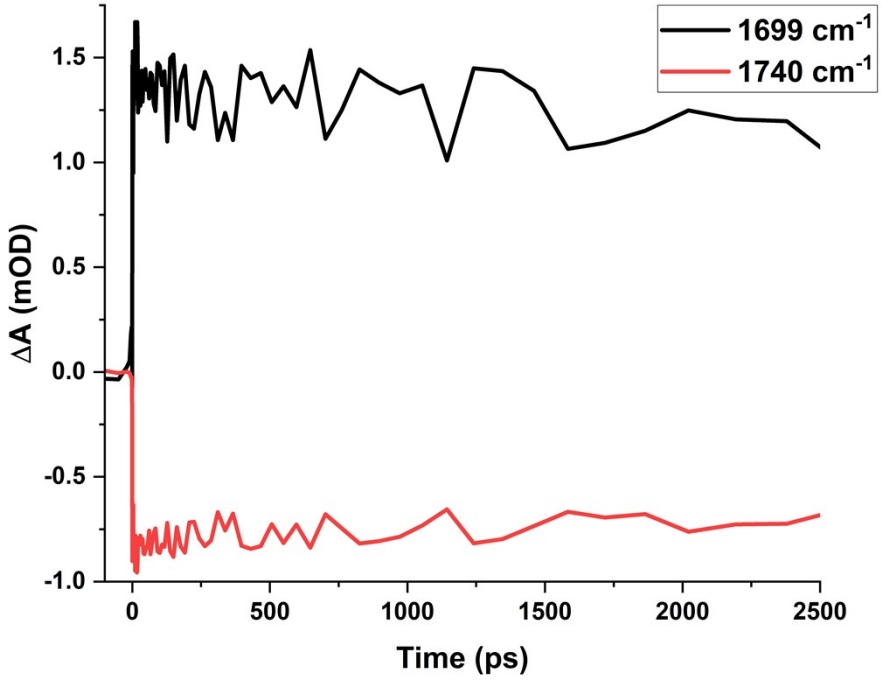

Figure S11. TRIR kinetics of [Cu(xant)(deebq)]BF_4 (**D2**). TRIR spectra were recorded in DCM following excitation at 500 nm (2 mW, OD@500nm = 0.6), collected with the pump set to magic angle (54.7 ˚) with respect to the probe.

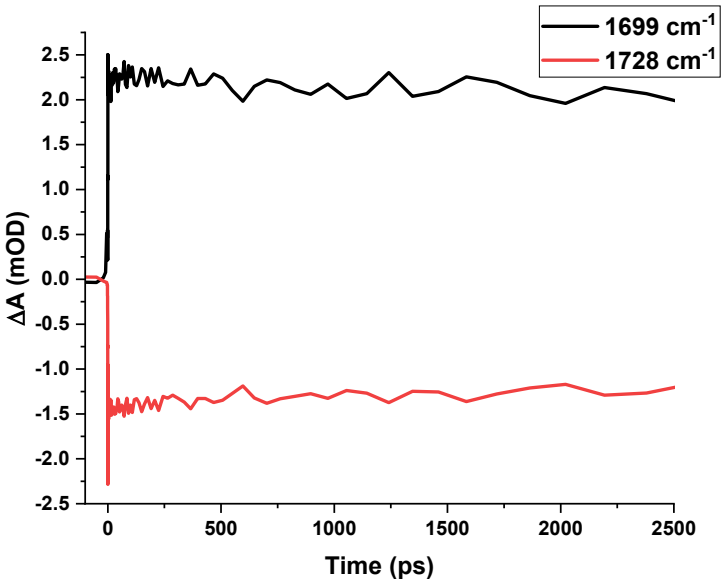

Figure S12. TRIR spectra of [Cu(DPEphos)(deebq)]BF_4 (D3) from 1340-1620 cm^{-1}. TRIR spectra were recorded in DCM following excitation at 530 nm (2 mW, OD@530nm = 0.65), collected with the pump set to magic angle (54.7 ˚) with respect to the probe. The time delay between the pump and probe for each spectrum is shown in the legend.

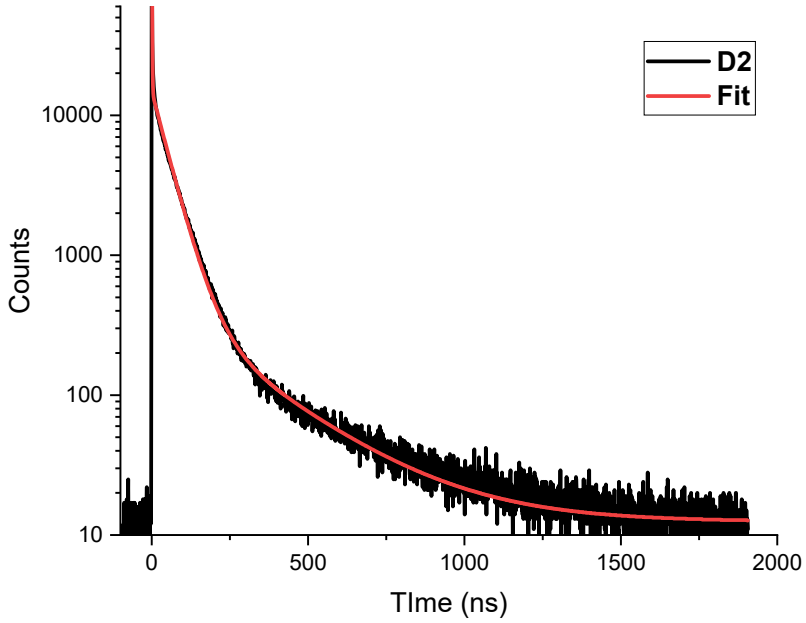

Figure S13. TCSPC data for emission decay of D2 in aerated DCM (405 nm excitation), collected with 50-nm band-pass filter.

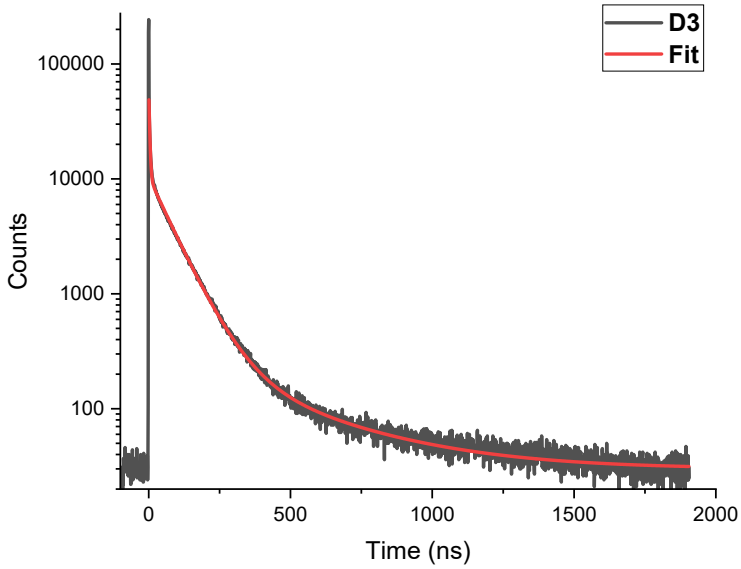

Figure S14. TSCPC for emission decay of D3 in aerated DCM (405 nm excitation), collected with 50-nm band-pass filter.

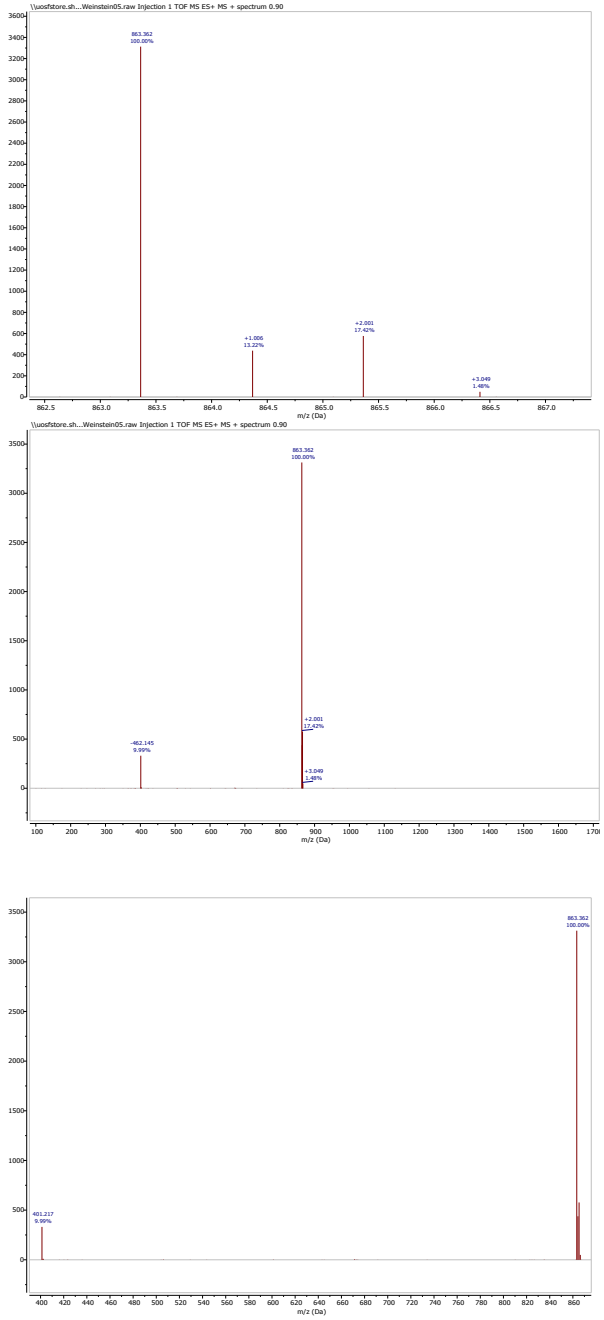

Figure S15. ES+ Mass Spectra of **D1** (note that only one species with Cu is present)

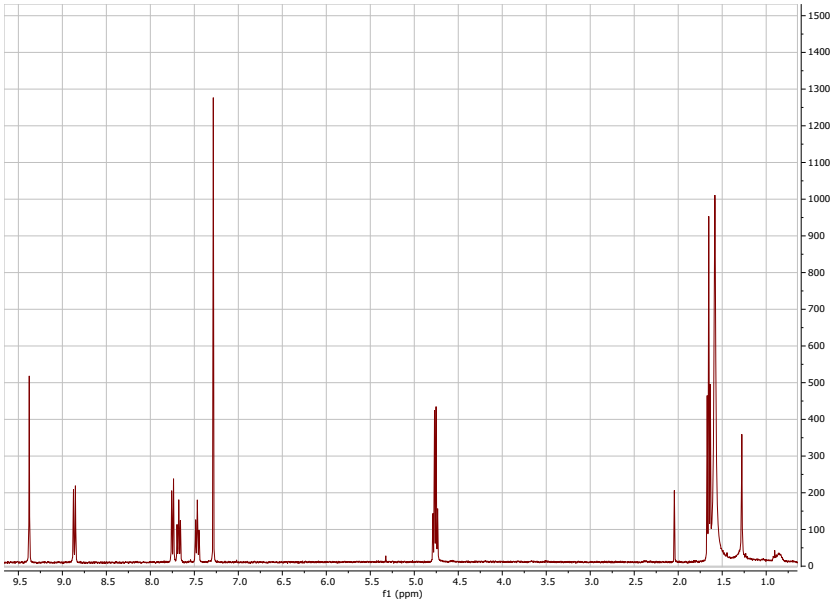

Figure S16: ^{1}H NMR of complex **D1** in $CDCl_3$. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm): 9.38 (4H, s), 8.86 (4H, d, J=8.0 Hz), 7.73 (4H, d, J=8.5 Hz), 7.68 (4H, t, J=7.5 Hz), 7.45 (4H, t, J=7.5 Hz), 4.76 (8H, q, J=7.4 Hz), 1.58 (12H, t, J=7.1 Hz).

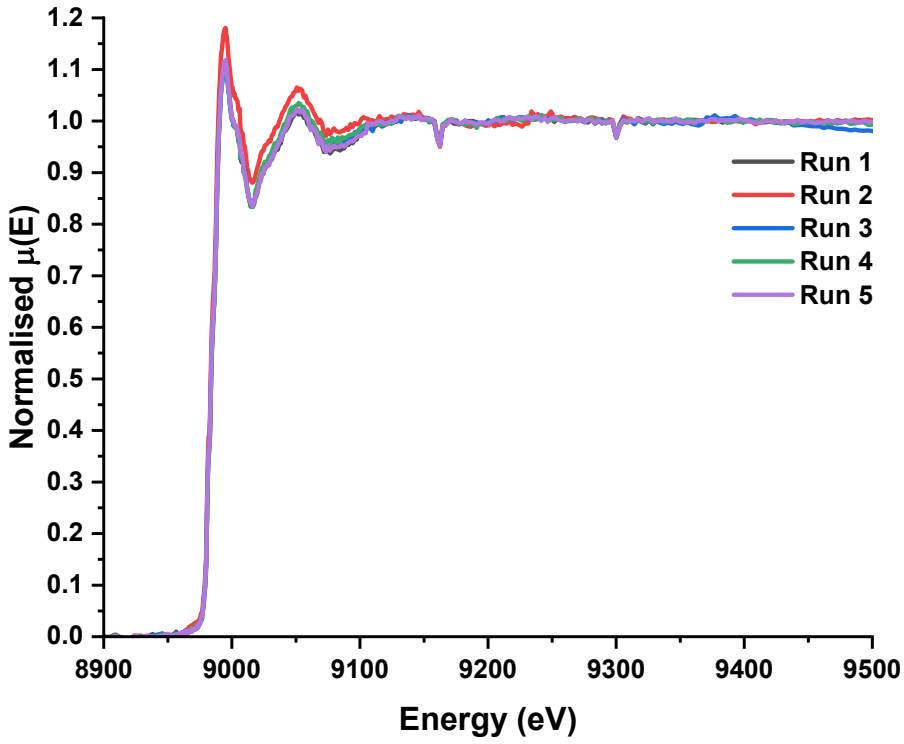

Figure S17. Sequential runs of EXAFS recorded for D1 plotted as normalised m(E) against energy, eV, showing no major changes to the spectra following repeated X-ray exposure. Run 2 (red spectrum) is slightly higher in intensity – note that the data are not normalised for the X-ray flux.

4. Crystallography data for complex **D1**

Table S2 Crystal data and structure refinement for D1.

Identification code	**D1**
Empirical formula	$C_{48}H_{40}BCuF_4N_4O_8$
Formula weight	951.19
Temperature/K	100.00
Crystal system	triclinic
Space group	P-1
a/Å	11.7561(8)
b/Å	13.8748(10)
c/Å	14.2785(10)
α/°	88.744(3)
β/°	75.329(4)
γ/°	66.116(3)
Volume/Å^3	2051.6(3)
Z	2
ρ_{calc}g/cm^3	1.540
μ/mm^{-1}	1.459
F(000)	980.0
Crystal size/mm^3	0.25 × 0.084 × 0.068
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	6.426 to 133.914
Index ranges	-13 ≤ h ≤ 14, -16 ≤ k ≤ 16, -16 ≤ l ≤ 17
Reflections collected	26569
Independent reflections	7071 [R_{int} = 0.0790, R_{sigma} = 0.0586]
Data/restraints/parameters	7071/0/599
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0902, wR_2 = 0.2439
Final R indexes [all data]	R_1 = 0.1225, wR_2 = 0.2747
Largest diff. peak/hole / e Å^{-3}	1.53/-0.49

Table S3 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for D1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu1	6981.9(8)	6279.3(6)	3060.5(6)	45.5(3)
F1	9434(3)	1724(3)	4201(2)	56.1(8)
F2	10321(3)	1018(3)	2621(3)	60.5(9)
F3	8194(3)	1447(3)	3333(3)	54.7(8)
F4	8914(4)	2743(3)	2970(3)	59.2(9)

Table S3 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for D1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	5204(5)	2106(3)	2545(3)	57.5(11)
O2	5116(4)	2184(3)	4135(3)	50.1(9)
O3	9069(5)	3821(4)	7113(3)	57.5(11)
O4	8210(4)	2858(3)	6542(3)	53.2(10)
O5	3707(4)	11222(3)	1352(3)	59.8(11)
O6	5809(4)	10713(3)	646(3)	50.7(9)
O7	12577(4)	6129(4)	-469(3)	65.2(12)
O8	11048(4)	7770(3)	-363(3)	51.9(10)
N1	6127(4)	5265(4)	3146(3)	43.5(10)
N2	7353(5)	5637(3)	4289(3)	43.8(10)
N3	6190(5)	7789(4)	2740(3)	45.2(10)
N4	8461(5)	6232(4)	1920(3)	44.4(10)
C1	5449(5)	5140(4)	2534(4)	43.0(12)
C2	5123(6)	5909(4)	1853(4)	47.1(13)
C3	4453(6)	5821(5)	1240(4)	50.2(13)
C4	4023(6)	5005(5)	1288(4)	52.5(14)
C5	4326(6)	4253(5)	1929(4)	49.1(13)
C6	5057(5)	4292(4)	2564(4)	45.5(12)
C7	5423(5)	3550(4)	3258(4)	44.1(12)
C8	6035(5)	3723(4)	3892(4)	44.8(12)
C9	6392(5)	4584(4)	3808(4)	40.9(11)
C10	7088(5)	4795(4)	4467(4)	42.9(12)
C11	7450(5)	4159(4)	5207(4)	44.0(12)
C12	8045(5)	4430(4)	5815(4)	44.4(12)
C13	8260(6)	5367(4)	5686(4)	44.9(12)
C14	8782(6)	5777(5)	6295(4)	50.0(13)
C15	8980(6)	6675(5)	6096(4)	50.8(13)
C16	8685(6)	7212(5)	5281(4)	49.3(13)
C17	8154(6)	6861(4)	4697(4)	45.8(12)
C18	7915(5)	5947(4)	4884(4)	44.5(12)
C19	5223(6)	2554(5)	3256(4)	48.7(13)
C20	5037(6)	1162(5)	4181(4)	52.5(14)
C21	6329(6)	270(5)	3804(5)	54.2(14)
C22	8500(6)	3686(5)	6573(4)	47.7(13)
C23	8693(6)	2052(5)	7188(4)	54.1(14)
C24	10081(7)	1336(5)	6777(5)	67.6(18)
C25	4932(6)	8486(4)	3060(4)	45.4(12)
C26	4141(6)	8207(4)	3830(4)	44.8(12)
C27	2860(6)	8863(5)	4202(4)	50.0(13)
C28	2332(6)	9839(5)	3806(4)	48.1(13)
C29	3083(6)	10143(5)	3056(4)	48.1(13)

Table S3 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for D1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C30	4394(6)	9481(4)	2653(4)	44.3(12)
C31	5271(6)	9693(5)	1859(4)	49.4(13)
C32	6523(6)	8988(5)	1561(4)	46.0(12)
C33	6964(6)	8032(4)	2003(4)	43.9(12)
C34	8288(6)	7193(4)	1633(4)	44.8(12)
C35	9299(6)	7361(5)	964(4)	44.5(12)
C36	10442(6)	6545(5)	556(4)	44.1(12)
C37	10624(5)	5486(4)	787(4)	43.2(12)
C38	11713(6)	4551(5)	362(4)	46.7(12)
C39	11794(6)	3587(4)	659(4)	47.6(13)
C40	10794(6)	3486(5)	1386(4)	46.7(12)
C41	9705(6)	4371(4)	1797(4)	46.4(12)
C42	9592(6)	5388(4)	1510(4)	45.4(12)
C43	4799(6)	10641(5)	1298(4)	48.0(13)
C44	5498(6)	11541(5)	-2(4)	50.6(13)
C45	6689(6)	11289(5)	-832(4)	53.0(14)
C46	11478(6)	6772(5)	-155(4)	47.9(13)
C47	11969(6)	8052(5)	-1089(4)	49.8(13)
C48	11375(6)	9239(5)	-1095(4)	52.6(14)
B1	9224(7)	1726(5)	3270(5)	48.9(15)

Table S4 Anisotropic Displacement Parameters (Å^2×10^3) for D1. 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}
Cu1	52.3(5)	47.3(5)	38.9(5)	9.8(3)	-11.7(4)	-23.1(4)
F1	60(2)	63(2)	44.4(18)	5.9(15)	-14.7(15)	-24.8(17)
F2	53(2)	68(2)	49.0(19)	3.6(16)	-9.6(16)	-16.7(17)
F3	59(2)	54.5(19)	54.7(19)	8.5(15)	-14.7(16)	-27.8(16)
F4	60(2)	59(2)	63(2)	16.8(16)	-15.1(17)	-30.7(17)
O1	80(3)	57(2)	47(2)	5.5(18)	-21(2)	-36(2)
O2	62(2)	54(2)	41(2)	8.2(17)	-10.7(18)	-32(2)
O3	74(3)	65(3)	53(2)	19(2)	-32(2)	-40(2)
O4	70(3)	56(2)	43(2)	15.5(18)	-19.4(19)	-33(2)
O5	50(3)	59(3)	64(3)	22(2)	-14(2)	-18(2)
O6	57(2)	55(2)	41(2)	15.2(17)	-14.1(18)	-23.2(19)
O7	56(3)	59(3)	65(3)	20(2)	-4(2)	-16(2)
O8	53(2)	54(2)	45(2)	11.3(17)	-5.7(18)	-22.5(19)
N1	47(3)	47(2)	38(2)	8.9(18)	-9.6(19)	-21(2)
N2	50(3)	42(2)	39(2)	6.5(18)	-9(2)	-21(2)
N3	50(3)	45(2)	45(2)	8.1(19)	-15(2)	-23(2)

Table S4 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for D1. 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}
N4	54(3)	48(3)	35(2)	8.3(18)	-15(2)	-23(2)
C1	44(3)	46(3)	37(3)	1(2)	-11(2)	-16(2)
C2	55(3)	45(3)	40(3)	9(2)	-8(2)	-21(3)
C3	60(4)	52(3)	40(3)	9(2)	-17(3)	-22(3)
C4	55(3)	59(4)	41(3)	2(3)	-13(3)	-21(3)
C5	54(3)	54(3)	41(3)	3(2)	-10(3)	-26(3)
C6	46(3)	49(3)	39(3)	6(2)	-5(2)	-20(2)
C7	45(3)	44(3)	42(3)	5(2)	-8(2)	-20(2)
C8	47(3)	48(3)	36(3)	7(2)	-9(2)	-18(2)
C9	45(3)	38(3)	37(3)	6(2)	-9(2)	-15(2)
C10	44(3)	44(3)	36(3)	4(2)	-6(2)	-17(2)
C11	46(3)	47(3)	37(3)	3(2)	-7(2)	-19(2)
C12	43(3)	49(3)	39(3)	7(2)	-9(2)	-18(2)
C13	48(3)	49(3)	38(3)	7(2)	-10(2)	-21(2)
C14	58(3)	55(3)	44(3)	10(2)	-16(3)	-28(3)
C15	52(3)	58(3)	51(3)	4(3)	-16(3)	-30(3)
C16	57(3)	49(3)	48(3)	7(2)	-14(3)	-28(3)
C17	50(3)	43(3)	42(3)	7(2)	-13(2)	-17(2)
C18	41(3)	50(3)	40(3)	4(2)	-4(2)	-20(2)
C19	51(3)	56(3)	45(3)	10(3)	-15(3)	-27(3)
C20	66(4)	59(3)	40(3)	7(2)	-10(3)	-36(3)
C21	68(4)	55(3)	50(3)	14(3)	-22(3)	-32(3)
C22	50(3)	52(3)	42(3)	5(2)	-9(3)	-24(3)
C23	66(4)	56(3)	47(3)	17(3)	-20(3)	-31(3)
C24	74(5)	57(4)	63(4)	19(3)	-5(3)	-26(3)
C25	49(3)	48(3)	41(3)	5(2)	-15(2)	-21(2)
C26	54(3)	43(3)	38(3)	8(2)	-11(2)	-22(2)
C27	55(3)	57(3)	42(3)	9(2)	-13(3)	-28(3)
C28	49(3)	53(3)	40(3)	4(2)	-9(2)	-20(3)
C29	54(3)	48(3)	40(3)	4(2)	-14(2)	-18(3)
C30	55(3)	47(3)	36(3)	7(2)	-17(2)	-24(3)
C31	60(4)	50(3)	40(3)	6(2)	-14(3)	-24(3)
C32	48(3)	52(3)	43(3)	5(2)	-11(2)	-26(3)
C33	49(3)	44(3)	42(3)	9(2)	-12(2)	-23(2)
C34	50(3)	46(3)	41(3)	11(2)	-12(2)	-23(2)
C35	53(3)	51(3)	33(3)	9(2)	-13(2)	-25(3)
C36	49(3)	54(3)	33(3)	10(2)	-15(2)	-23(3)
C37	44(3)	52(3)	36(3)	7(2)	-13(2)	-21(2)
C38	51(3)	56(3)	34(3)	6(2)	-14(2)	-22(3)
C39	53(3)	42(3)	46(3)	2(2)	-19(3)	-15(2)
C40	55(3)	49(3)	41(3)	7(2)	-20(3)	-24(3)
C41	54(3)	46(3)	39(3)	9(2)	-14(2)	-20(3)

Table S4 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for D1. 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}
C42	55(3)	46(3)	38(3)	11(2)	-18(2)	-22(3)
C43	56(4)	49(3)	43(3)	8(2)	-16(3)	-24(3)
C44	58(3)	49(3)	48(3)	14(2)	-17(3)	-24(3)
C45	65(4)	57(3)	40(3)	13(3)	-13(3)	-29(3)
C46	47(3)	52(3)	42(3)	8(2)	-12(2)	-18(3)
C47	50(3)	56(3)	40(3)	7(2)	-2(2)	-25(3)
C48	60(4)	57(3)	42(3)	8(3)	-9(3)	-29(3)
B1	49(4)	52(4)	47(3)	12(3)	-16(3)	-21(3)

Table S5 Bond Lengths for D1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	N1	2.019(4)	C8	C9	1.412(8)
Cu1	N2	2.016(5)	C9	C10	1.495(8)
Cu1	N3	2.015(5)	C10	C11	1.400(8)
Cu1	N4	2.040(5)	C11	C12	1.385(8)
F1	B1	1.411(8)	C12	C13	1.422(8)
F2	B1	1.377(8)	C12	C22	1.524(8)
F3	B1	1.396(8)	C13	C14	1.425(8)
F4	B1	1.394(7)	C13	C18	1.433(8)
O1	C19	1.212(7)	C14	C15	1.369(8)
O2	C19	1.340(7)	C15	C16	1.410(8)
O2	C20	1.457(7)	C16	C17	1.361(8)
O3	C22	1.203(7)	C17	C18	1.412(8)
O4	C22	1.329(7)	C20	C21	1.490(9)
O4	C23	1.460(7)	C23	C24	1.491(10)
O5	C43	1.191(7)	C25	C26	1.406(8)
O6	C43	1.348(7)	C25	C30	1.445(8)
O6	C44	1.446(6)	C26	C27	1.374(9)
O7	C46	1.207(7)	C27	C28	1.415(8)
O8	C46	1.324(7)	C28	C29	1.381(8)
O8	C47	1.469(6)	C29	C30	1.406(8)
N1	C1	1.380(7)	C30	C31	1.440(8)
N1	C9	1.325(7)	C31	C32	1.356(9)
N2	C10	1.330(7)	C31	C43	1.506(8)
N2	C18	1.369(7)	C32	C33	1.414(8)
N3	C25	1.360(8)	C33	C34	1.484(8)
N3	C33	1.341(7)	C34	C35	1.420(8)
N4	C34	1.336(7)	C35	C36	1.352(8)
N4	C42	1.362(8)	C36	C37	1.440(8)
C1	C2	1.429(8)	C36	C46	1.512(8)

Table S5 Bond Lengths for D1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C6	1.423(8)	C37	C38	1.409(8)
C2	C3	1.354(8)	C37	C42	1.432(8)
C3	C4	1.408(9)	C38	C39	1.368(8)
C4	C5	1.369(8)	C39	C40	1.410(8)
C5	C6	1.414(8)	C40	C41	1.368(8)
C6	C7	1.428(8)	C41	C42	1.424(8)
C7	C8	1.368(8)	C44	C45	1.507(9)
C7	C19	1.494(8)	C47	C48	1.507(8)

Table S6 Bond Angles for D1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Cu1	N4	123.94(18)	O1	C19	O2	123.5(5)
N2	Cu1	N1	80.76(18)	O1	C19	C7	124.7(5)
N2	Cu1	N4	120.00(19)	O2	C19	C7	111.7(5)
N3	Cu1	N1	124.12(19)	O2	C20	C21	111.8(5)
N3	Cu1	N2	132.49(19)	O3	C22	O4	124.7(5)
N3	Cu1	N4	81.66(19)	O3	C22	C12	124.4(5)
C19	O2	C20	115.5(4)	O4	C22	C12	110.9(5)
C22	O4	C23	115.4(5)	O4	C23	C24	112.2(5)
C43	O6	C44	116.2(5)	N3	C25	C26	117.1(5)
C46	O8	C47	115.8(4)	N3	C25	C30	123.2(5)
C1	N1	Cu1	127.3(4)	C26	C25	C30	119.8(5)
C9	N1	Cu1	113.7(4)	C27	C26	C25	121.1(5)
C9	N1	C1	118.5(5)	C26	C27	C28	119.2(5)
C10	N2	Cu1	114.2(4)	C29	C28	C27	121.2(6)
C10	N2	C18	119.7(5)	C28	C29	C30	120.8(5)
C18	N2	Cu1	126.0(3)	C29	C30	C25	117.9(5)
C25	N3	Cu1	127.0(4)	C29	C30	C31	126.3(5)
C33	N3	Cu1	113.5(4)	C31	C30	C25	115.9(5)
C33	N3	C25	118.4(5)	C30	C31	C43	121.1(5)
C34	N4	Cu1	112.1(4)	C32	C31	C30	119.6(5)
C34	N4	C42	119.4(5)	C32	C31	C43	119.1(5)
C42	N4	Cu1	128.2(4)	C31	C32	C33	120.6(5)
N1	C1	C2	117.7(5)	N3	C33	C32	122.3(5)
N1	C1	C6	122.7(5)	N3	C33	C34	115.3(5)
C6	C1	C2	119.5(5)	C32	C33	C34	122.2(5)
C3	C2	C1	119.8(5)	N4	C34	C33	115.6(5)
C2	C3	C4	121.0(5)	N4	C34	C35	121.0(5)
C5	C4	C3	120.5(6)	C35	C34	C33	123.3(5)
C4	C5	C6	120.5(5)	C36	C35	C34	121.1(5)
C1	C6	C7	116.4(5)	C35	C36	C37	119.3(5)

Table S6 Bond Angles for D1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C5	C6	C1	118.5(5)	C35	C36	C46	118.7(5)
C5	C6	C7	125.0(5)	C37	C36	C46	122.0(5)
C6	C7	C19	120.6(5)	C38	C37	C36	125.9(5)
C8	C7	C6	119.7(5)	C38	C37	C42	117.9(5)
C8	C7	C19	119.6(5)	C42	C37	C36	116.2(5)
C7	C8	C9	120.0(5)	C39	C38	C37	120.7(5)
N1	C9	C8	122.4(5)	C38	C39	C40	121.8(6)
N1	C9	C10	115.3(5)	C41	C40	C39	119.3(5)
C8	C9	C10	122.2(5)	C40	C41	C42	120.4(5)
N2	C10	C9	114.5(5)	N4	C42	C37	122.7(5)
N2	C10	C11	122.1(5)	N4	C42	C41	117.4(5)
C11	C10	C9	123.3(5)	C41	C42	C37	119.9(5)
C12	C11	C10	120.0(5)	O5	C43	O6	122.9(5)
C11	C12	C13	119.2(5)	O5	C43	C31	127.1(5)
C11	C12	C22	118.7(5)	O6	C43	C31	109.9(5)
C13	C12	C22	122.0(5)	O6	C44	C45	107.2(5)
C12	C13	C14	125.2(5)	O7	C46	O8	124.1(5)
C12	C13	C18	117.3(5)	O7	C46	C36	123.9(5)
C14	C13	C18	117.6(5)	O8	C46	C36	111.9(5)
C15	C14	C13	120.7(5)	O8	C47	C48	107.1(5)
C14	C15	C16	121.0(5)	F2	B1	F1	109.9(5)
C17	C16	C15	120.1(5)	F2	B1	F3	110.3(5)
C16	C17	C18	120.8(5)	F2	B1	F4	109.8(5)
N2	C18	C13	121.5(5)	F3	B1	F1	108.6(5)
N2	C18	C17	118.7(5)	F4	B1	F1	108.7(5)
C17	C18	C13	119.8(5)	F4	B1	F3	109.4(5)

Table S7 Torsion Angles for D1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu1	N1	C1	C2	-10.9(7)	C16	C17	C18	N2	178.6(5)
Cu1	N1	C1	C6	169.8(4)	C16	C17	C18	C13	-1.3(9)
Cu1	N1	C9	C8	-171.2(4)	C18	N2	C10	C9	175.9(5)
Cu1	N1	C9	C10	9.2(6)	C18	N2	C10	C11	-4.8(8)
Cu1	N2	C10	C9	-8.4(6)	C18	C13	C14	C15	-2.0(9)
Cu1	N2	C10	C11	170.8(4)	C19	O2	C20	C21	78.6(6)
Cu1	N2	C18	C13	-173.4(4)	C19	C7	C8	C9	171.0(5)
Cu1	N2	C18	C17	6.7(7)	C20	O2	C19	O1	3.0(9)
Cu1	N3	C25	C26	12.8(7)	C20	O2	C19	C7	-174.6(5)
Cu1	N3	C25	C30	-167.7(4)	C22	O4	C23	C24	-80.1(7)
Cu1	N3	C33	C32	169.5(4)	C22	C12	C13	C14	-7.0(9)
Cu1	N3	C33	C34	-6.0(6)	C22	C12	C13	C18	173.4(5)

Table S7 Torsion Angles for D1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu1	N4	C34	C33	-14.9(6)	C23	O4	C22	O3	-3.3(9)
Cu1	N4	C34	C35	169.2(4)	C23	O4	C22	C12	175.4(5)
Cu1	N4	C42	C37	-172.1(4)	C25	N3	C33	C32	0.9(8)
Cu1	N4	C42	C41	10.6(7)	C25	N3	C33	C34	-174.5(5)
N1	C1	C2	C3	-179.7(5)	C25	C26	C27	C28	-0.4(9)
N1	C1	C6	C5	177.8(5)	C25	C30	C31	C32	-1.8(8)
N1	C1	C6	C7	-1.0(8)	C25	C30	C31	C43	173.0(5)
N1	C9	C10	N2	-0.5(7)	C26	C25	C30	C29	0.4(8)
N1	C9	C10	C11	-179.8(5)	C26	C25	C30	C31	-179.2(5)
N2	C10	C11	C12	3.5(8)	C26	C27	C28	C29	-0.2(9)
N3	C25	C26	C27	179.8(5)	C27	C28	C29	C30	1.0(9)
N3	C25	C30	C29	-179.1(5)	C28	C29	C30	C25	-1.0(8)
N3	C25	C30	C31	1.3(8)	C28	C29	C30	C31	178.5(5)
N3	C33	C34	N4	14.3(7)	C29	C30	C31	C32	178.6(5)
N3	C33	C34	C35	-169.9(5)	C29	C30	C31	C43	-6.6(9)
N4	C34	C35	C36	3.8(8)	C30	C25	C26	C27	0.3(8)
C1	N1	C9	C8	1.7(8)	C30	C31	C32	C33	2.0(8)
C1	N1	C9	C10	-177.9(5)	C30	C31	C43	O5	-9.2(9)
C1	C2	C3	C4	2.6(9)	C30	C31	C43	O6	175.2(5)
C1	C6	C7	C8	4.5(8)	C31	C32	C33	N3	-1.5(9)
C1	C6	C7	C19	-171.5(5)	C31	C32	C33	C34	173.6(5)
C2	C1	C6	C5	-1.5(8)	C32	C31	C43	O5	165.6(6)
C2	C1	C6	C7	179.7(5)	C32	C31	C43	O6	-9.9(7)
C2	C3	C4	C5	-3.0(9)	C32	C33	C34	N4	-161.1(5)
C3	C4	C5	C6	1.0(9)	C32	C33	C34	C35	14.7(9)
C4	C5	C6	C1	1.2(9)	C33	N3	C25	C26	179.6(5)
C4	C5	C6	C7	179.9(6)	C33	N3	C25	C30	-0.9(8)
C5	C6	C7	C8	-174.3(6)	C33	C34	C35	C36	-171.8(5)
C5	C6	C7	C19	9.8(9)	C34	N4	C42	C37	0.8(8)
C6	C1	C2	C3	-0.4(9)	C34	N4	C42	C41	-176.5(5)
C6	C7	C8	C9	-4.9(8)	C34	C35	C36	C37	1.5(8)
C6	C7	C19	O1	27.7(9)	C34	C35	C36	C46	179.6(5)
C6	C7	C19	O2	-154.8(5)	C35	C36	C37	C38	174.5(5)
C7	C8	C9	N1	1.8(8)	C35	C36	C37	C42	-5.1(7)
C7	C8	C9	C10	-178.6(5)	C35	C36	C46	O7	170.7(6)
C8	C7	C19	O1	-148.3(6)	C35	C36	C46	O8	-7.0(7)
C8	C7	C19	O2	29.2(8)	C36	C37	C38	C39	178.2(5)
C8	C9	C10	N2	179.9(5)	C36	C37	C42	N4	4.1(8)
C8	C9	C10	C11	0.6(8)	C36	C37	C42	C41	-178.6(5)
C9	N1	C1	C2	177.3(5)	C37	C36	C46	O7	-11.2(9)
C9	N1	C1	C6	-2.0(8)	C37	C36	C46	O8	171.2(5)
C9	C10	C11	C12	-177.3(5)	C37	C38	C39	C40	0.9(9)
C10	N2	C18	C13	1.7(8)	C38	C37	C42	N4	-175.5(5)

Table S7 Torsion Angles for D1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C10	N2	C18	C17	-178.2(5)	C38	C37	C42	C41	1.7(8)
C10	C11	C12	C13	1.1(8)	C38	C39	C40	C41	0.9(8)
C10	C11	C12	C22	-176.3(5)	C39	C40	C41	C42	-1.3(8)
C11	C12	C13	C14	175.7(5)	C40	C41	C42	N4	177.4(5)
C11	C12	C13	C18	-3.9(8)	C40	C41	C42	C37	0.0(8)
C11	C12	C22	O3	177.2(6)	C42	N4	C34	C33	171.0(5)
C11	C12	C22	O4	-1.5(7)	C42	N4	C34	C35	-4.9(8)
C12	C13	C14	C15	178.5(6)	C42	C37	C38	C39	-2.2(8)
C12	C13	C18	N2	2.6(8)	C43	O6	C44	C45	-163.8(5)
C12	C13	C18	C17	-177.5(5)	C43	C31	C32	C33	-173.0(5)
C13	C12	C22	O3	-0.2(9)	C44	O6	C43	O5	-0.4(8)
C13	C12	C22	O4	-178.8(5)	C44	O6	C43	C31	175.4(5)
C13	C14	C15	C16	-0.6(10)	C46	O8	C47	C48	-170.8(5)
C14	C13	C18	N2	-177.0(5)	C46	C36	C37	C38	-3.7(8)
C14	C13	C18	C17	2.9(8)	C46	C36	C37	C42	176.8(5)
C14	C15	C16	C17	2.3(9)	C47	O8	C46	O7	5.5(9)
C15	C16	C17	C18	-1.3(9)	C47	O8	C46	C36	-176.9(5)

Table S8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for D1.

Atom	*x*	*y*	*z*	U(eq)
H2	5376.22	6480.49	1830.55	57
H3	4269.7	6316.89	770.64	60
H4	3518.56	4976.82	873.19	63
H5	4041.57	3699.97	1946.92	59
H8	6219.61	3262.51	4387.86	54
H11	7286.92	3541.04	5292.5	53
H14	8994.8	5423.45	6844.72	60
H15	9321.3	6940.68	6513.97	61
H16	8857.67	7819.24	5139.42	59
H17	7941.14	7234.87	4156.38	55
H20A	4455.21	1143.66	3794.03	63
H20B	4662.02	1074.31	4863.66	63
H21A	6687.06	338.9	3120.49	81
H21B	6240.04	-402.86	3860.59	81
H21C	6907.91	287.69	4184.58	81
H23A	8176.61	1626.35	7305.52	65
H23B	8583.49	2402.55	7821.64	65
H24A	10212.72	1054.69	6115.99	101
H24B	10332.62	749.17	7184.87	101
H24C	10610.61	1732.59	6759.98	101

Table S8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for D1.

Atom	*x*	*y*	*z*	U(eq)
H26	4499.93	7553.07	4097.25	54
H27	2333.38	8664.31	4719.95	60
H28	1444.95	10293.28	4060.2	58
H29	2709.57	10806.5	2808.74	58
H32	7108.1	9137.26	1050.94	55
H35	9169.03	8058.35	801.69	53
H38	12398.09	4591.44	-136.1	56
H39	12543.74	2969.62	368.42	57
H40	10876.39	2808.99	1587.53	56
H41	9019.53	4307.14	2277.6	56
H44A	5244.14	12237.29	345.05	61
H44B	4771.84	11565.57	-247.12	61
H45A	6470.5	11755.6	-1344.88	79
H45B	7022.13	10550.02	-1093.11	79
H45C	7348.07	11396.82	-599.74	79
H47A	12133.62	7708.95	-1738.98	60
H47B	12799.32	7816.04	-915.81	60
H48A	11968.02	9458.68	-1567.91	79
H48B	11209.65	9568.87	-446.06	79
H48C	10559.4	9461.6	-1273.86	79

4.1. Crystal structure determination of D1

Crystal Data for $C_{48}H_{40}BCuF_4N_4O_8$ (M =951.19 g/mol): triclinic, space group P-1 (no. 2), a = 11.7561(8) Å, b = 13.8748(10) Å, c = 14.2785(10) Å, α = 88.744(3)°, β = 75.329(4)°, γ = 66.116(3)°, V = 2051.6(3) Å^3, Z = 2, T = 100.00 K, μ(CuKα) = 1.459 mm^{-1}, *Dcalc* = 1.540 g/cm^3, 26569 reflections measured (6.426° ≤ 2Θ ≤ 133.914°), 7071 unique (R_{int} = 0.0790, R_{sigma} = 0.0586) which were used in all calculations. The final R_1 was 0.0902 (I > 2σ(I)) and wR_2 was 0.2747 (all data).

5. Crystallography data for complex **D2**

Table S9 Crystal data and structure refinement for D2.

Identification code	**D2**
Empirical formula	$C_{63}H_{52}BCuF_4N_2O_5P_2$
Formula weight	1129.35
Temperature/K	100.00
Crystal system	triclinic
Space group	P-1
a/Å	11.2410(5)
b/Å	14.6532(8)
c/Å	18.4225(8)
α/°	73.672(3)
β/°	86.086(3)
γ/°	70.147(3)

Volume/Å^3	2737.8(2)
Z	2
ρ_{calc}g/cm^3	1.370
μ/mm^{-1}	1.668
F(000)	1168.0
Crystal size/mm^3	0.23 × 0.12 × 0.02
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	5 to 141.634
Index ranges	-13 ≤ h ≤ 12, -17 ≤ k ≤ 17, -22 ≤ l ≤ 22
Reflections collected	57710
Independent reflections	10363 [R_{int} = 0.1112, R_{sigma} = 0.0731]
Data/restraints/parameters	10363/890/911
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0962, wR_2 = 0.2518
Final R indexes [all data]	R_1 = 0.1429, wR_2 = 0.3004
Largest diff. peak/hole / e Å^{-3}	1.08/-0.81

Table S10 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for D2. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu1	1324.6(7)	4072.9(7)	2705.1(4)	42.3(3)
P1	3196.2(14)	2886.5(14)	3185.7(8)	50.1(4)
P2	-24.5(15)	3557.8(14)	2175.2(9)	51.0(4)
O1	2473(4)	2266(3)	1959(2)	49.5(10)
O2	2634(5)	8561(4)	732(4)	84.6(18)
O3	612(5)	9103(4)	1063(3)	73.3(15)
N1	1473(4)	5430(4)	2024(3)	44.8(11)
N2	291(5)	5058(5)	3327(3)	51.2(11)
C1	4173(6)	3347(6)	3651(3)	58.6(16)
C2	4022(7)	4347(7)	3414(4)	73.2(19)
C3	4727(7)	4769(9)	3722(5)	86(2)
C4	5584(8)	4157(10)	4309(5)	93(3)
C5	5703(10)	3213(12)	4570(6)	109(3)
C6	5004(8)	2783(9)	4257(4)	87(2)
C7	3110(7)	1724(7)	3850(4)	72.9(19)
C13	4261(6)	2408(5)	2474(3)	52.8(15)
C14	5552(6)	2312(7)	2440(4)	75(2)
C15	6257(7)	1990(7)	1853(4)	73(2)
C16	5720(6)	1774(6)	1300(4)	58.8(16)
C17	4438(6)	1873(5)	1307(4)	50.3(14)
C18	3761(6)	2168(5)	1907(3)	47.0(13)
C19	2400(6)	2401(6)	627(4)	59.2(16)

Table S10 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for D2. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C20	1699(7)	2837(8)	-31(4)	76(2)
C21	454(7)	3504(9)	-68(5)	87(3)
C22	-126(7)	3714(7)	593(4)	68(2)
C23	565(6)	3276(6)	1279(4)	52.2(14)
C24	1815(6)	2644(5)	1277(4)	50.6(14)
C25	3747(7)	1650(6)	719(4)	60.3(16)
C26	3707(9)	571(7)	1025(6)	90(3)
C27	4432(7)	1727(7)	-31(4)	68(2)
C28	-1642(6)	4450(7)	1947(4)	64.1(17)
C29	-2656(8)	4182(10)	1839(7)	115(4)
C30	-3911(8)	4905(11)	1731(7)	114(3)
C31	-4130(9)	5816(11)	1741(5)	110(3)
C32	-3135(8)	6125(10)	1829(5)	100(3)
C33	-1902(7)	5427(8)	1928(4)	76(2)
C40	2158(5)	5595(5)	1378(3)	43.2(12)
C41	2713(5)	4776(5)	1061(3)	43.3(12)
C42	3340(6)	4908(5)	399(4)	47.5(13)
C43	3477(6)	5843(5)	41(4)	52.6(15)
C44	2947(6)	6653(5)	331(4)	52.1(14)
C45	2265(6)	6548(5)	1009(4)	49.7(14)
C46	1610(7)	7366(6)	1325(5)	65.3(18)
C47	923(9)	7172(6)	1963(6)	83(3)
C48	841(7)	6208(6)	2293(4)	61.4(17)
C49	1703(8)	8402(6)	998(5)	70(2)
C50	635(8)	10134(6)	883(6)	74(2)
C51	-696(8)	10788(6)	978(6)	80(2)
O4A	-3839(12)	7492(10)	3993(8)	120(5)
O5A	-3740(20)	7860(20)	2847(12)	229(12)
C8A	2827(13)	1817(13)	4666(7)	87(4)
C9A	2622(15)	1010(15)	5204(9)	105(5)
C10A	2681(16)	153(15)	4984(9)	105(5)
C11A	2770(30)	161(16)	4206(12)	125(8)
C12A	3092(17)	958(12)	3699(8)	94(4)
C34A	90(20)	2200(20)	2944(16)	43(5)
C35A	450(30)	1270(20)	2792(18)	48(6)
C36A	410(30)	370(30)	3314(19)	67(8)
C37A	20(30)	410(20)	4027(18)	65(7)
C38A	-380(30)	1330(20)	4197(16)	59(6)
C39A	-370(30)	2170(20)	3684(15)	54(6)
C52A	-77(14)	6012(9)	2882(8)	59(5)
C53A	-1188(14)	6828(12)	2942(9)	81(4)

Table S10 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for D2. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C54A	-1962(13)	6626(11)	3511(8)	78(4)
C55A	-1601(12)	5677(11)	4054(7)	56(3)
C56A	-2269(16)	5438(15)	4703(9)	66(5)
C57A	-1837(17)	4515(16)	5191(10)	61(5)
C58A	-745(15)	3759(13)	5046(8)	57(4)
C59A	-44(13)	3961(11)	4433(7)	49(3)
C60A	-500(20)	4920(11)	3917(13)	51(4)
C61A	-3176(19)	7515(16)	3548(11)	119(7)
C62A	-5270(20)	8624(17)	2744(13)	124(7)
C63A	-6260(30)	8350(20)	3359(15)	151(9)
O4B	-2444(19)	7248(15)	4892(10)	142(5)
O5B	-2770(20)	8276(16)	3542(12)	142(5)
C8B	1958(19)	1485(16)	3929(10)	62(5)
C9B	1860(30)	580(20)	4344(18)	97(9)
C10B	3030(30)	-230(30)	4540(18)	92(8)
C11B	4130(30)	-150(20)	4385(14)	92(7)
C12B	4210(20)	799(18)	3975(11)	76(6)
C34B	-414(12)	2483(9)	2665(7)	54(3)
C35B	41(12)	1567(9)	2492(7)	55(3)
C36B	-174(14)	711(10)	2931(9)	81(4)
C37B	-855(19)	782(13)	3586(11)	115(7)
C38B	-1300(20)	1679(13)	3796(11)	131(9)
C39B	-1122(18)	2545(12)	3325(9)	95(5)
C52B	222(15)	5999(10)	3029(9)	49(4)
C53B	-706(13)	6739(12)	3313(9)	58(3)
C54B	-1394(16)	6468(13)	3938(11)	74(4)
C55B	-1246(14)	5451(13)	4304(9)	55(3)
C56B	-1974(18)	5153(17)	4916(12)	59(5)
C57B	-1680(20)	4155(18)	5256(12)	61(5)
C58B	-760(30)	3417(17)	4968(11)	80(7)
C59B	-160(20)	3711(14)	4325(9)	63(5)
C60B	-320(30)	4736(14)	3991(14)	51(5)
C61B	-2230(30)	7280(20)	4299(15)	142(5)
C62B	-3590(30)	9556(19)	3413(16)	142(5)
C63B	-4480(30)	9440(20)	2797(17)	142(5)
F1	2392(15)	7035(7)	3225(6)	239(6)
F2	2152(12)	8166(7)	3887(5)	196(4)
F3	1996(9)	8693(5)	2543(4)	169(3)
F4	430(13)	8156(7)	3333(5)	182(4)
B1	1850(30)	7958(13)	3283(12)	170(5)

Table S11 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for D2. 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}
Cu1	37.6(5)	58.8(6)	30.8(4)	-20.5(4)	4.3(3)	-10.7(4)
P1	39.3(8)	72.4(11)	28.2(7)	-13.7(7)	4.7(6)	-6.3(7)
P2	45.8(8)	77.2(11)	48.7(9)	-38.2(8)	22.0(7)	-31.0(8)
O1	47(2)	59(3)	47(2)	-23.7(19)	19.5(17)	-19.0(18)
O2	64(3)	63(3)	144(5)	-52(3)	30(3)	-29(3)
O3	69(3)	52(3)	106(4)	-37(3)	31(3)	-22(2)
N1	38(2)	55(3)	47(2)	-29(2)	6.1(19)	-11(2)
N2	38(2)	82(3)	45(2)	-40(2)	5.6(19)	-17(2)
C1	36(3)	103(4)	31(3)	-27(3)	6(2)	-11(3)
C2	52(4)	112(5)	58(4)	-35(4)	-11(3)	-19(4)
C3	53(4)	148(7)	77(5)	-61(5)	3(3)	-34(4)
C4	52(4)	179(7)	64(5)	-66(5)	9(3)	-33(5)
C5	86(6)	180(8)	60(5)	-39(5)	-23(4)	-35(6)
C6	71(5)	133(6)	44(4)	-19(4)	-15(3)	-18(4)
C7	57(4)	82(4)	50(3)	3(3)	8(3)	-5(3)
C13	42(3)	70(4)	37(3)	-14(3)	8(2)	-9(3)
C14	39(3)	128(7)	51(4)	-36(4)	8(3)	-11(3)
C15	43(3)	103(6)	64(4)	-33(4)	15(3)	-9(3)
C16	49(3)	72(4)	51(3)	-23(3)	19(3)	-14(3)
C17	51(3)	50(3)	48(3)	-19(3)	19(2)	-15(3)
C18	40(3)	52(3)	44(3)	-13(2)	12(2)	-11(2)
C19	52(3)	91(4)	63(3)	-52(3)	27(2)	-39(3)
C20	56(3)	146(6)	61(4)	-69(4)	26(3)	-49(4)
C21	50(4)	174(8)	62(4)	-72(5)	16(3)	-40(4)
C22	48(3)	125(6)	56(3)	-56(4)	18(3)	-37(4)
C23	48(3)	82(4)	51(3)	-42(3)	21(2)	-37(3)
C24	48(3)	71(4)	52(3)	-36(3)	19(2)	-32(3)
C25	55(3)	79(4)	67(4)	-45(3)	32(3)	-33(3)
C26	93(6)	82(5)	125(7)	-62(4)	63(5)	-51(4)
C27	52(4)	108(6)	69(4)	-58(4)	30(3)	-36(4)
C28	36(3)	126(5)	49(3)	-57(3)	15(2)	-26(3)
C29	45(4)	190(8)	166(9)	-134(7)	36(4)	-48(4)
C30	38(4)	216(9)	126(8)	-118(7)	23(4)	-36(5)
C31	56(4)	208(9)	75(5)	-87(6)	5(4)	-17(5)
C32	54(4)	143(7)	84(6)	-41(5)	-15(4)	3(4)
C33	43(3)	125(5)	59(4)	-37(4)	-6(3)	-14(3)
C40	32(3)	54(3)	50(3)	-26(2)	3(2)	-13(2)
C41	33(3)	51(3)	51(3)	-24(2)	8(2)	-13(2)
C42	42(3)	50(3)	58(3)	-28(3)	16(3)	-16(2)
C43	41(3)	57(3)	63(4)	-24(3)	20(3)	-17(3)

Table S11 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for D2. 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}
C44	39(3)	51(3)	71(4)	-24(3)	11(3)	-16(3)
C45	37(3)	52(3)	66(3)	-25(3)	8(2)	-15(2)
C46	54(4)	56(3)	93(5)	-39(3)	18(3)	-16(3)
C47	91(6)	60(4)	106(5)	-48(4)	44(5)	-21(4)
C48	61(4)	61(3)	70(4)	-41(3)	22(3)	-15(3)
C49	62(4)	60(4)	100(5)	-42(3)	21(4)	-21(3)
C50	77(5)	52(4)	100(6)	-35(4)	26(4)	-22(3)
C51	77(5)	52(4)	102(6)	-26(4)	34(4)	-14(3)
O4A	78(7)	107(9)	118(8)	-7(7)	31(6)	15(6)
O5A	143(10)	280(20)	125(9)	-25(9)	10(7)	70(12)
C8A	74(8)	137(9)	52(5)	-20(5)	25(5)	-48(7)
C9A	100(11)	144(10)	66(7)	-12(6)	43(7)	-54(9)
C10A	93(10)	121(9)	71(7)	0(6)	28(7)	-25(8)
C11A	190(20)	92(10)	73(8)	-3(6)	39(9)	-43(12)
C12A	123(12)	81(6)	53(6)	-5(5)	23(6)	-16(7)
C34A	27(10)	69(8)	48(7)	-29(6)	10(6)	-28(7)
C35A	43(14)	67(9)	49(10)	-27(7)	9(9)	-29(8)
C36A	72(19)	69(10)	64(10)	-19(8)	21(10)	-33(10)
C37A	62(16)	77(11)	62(11)	-19(8)	19(10)	-35(10)
C38A	49(13)	77(10)	56(9)	-15(7)	7(8)	-32(9)
C39A	55(14)	69(10)	47(8)	-22(7)	11(8)	-30(9)
C52A	51(7)	79(5)	60(6)	-46(4)	11(6)	-19(4)
C53A	74(7)	93(7)	58(7)	-35(6)	19(6)	1(6)
C54A	63(6)	96(7)	50(6)	-30(5)	13(5)	10(5)
C55A	36(6)	95(6)	41(5)	-40(4)	-5(4)	-7(4)
C56A	40(8)	104(9)	49(6)	-39(5)	5(6)	-2(6)
C57A	41(7)	104(9)	40(6)	-47(7)	4(5)	-6(7)
C58A	46(6)	89(8)	40(6)	-37(5)	13(4)	-14(6)
C59A	38(5)	84(7)	37(5)	-41(5)	4(4)	-16(5)
C60A	34(7)	85(6)	42(5)	-39(4)	1(5)	-12(5)
C61A	91(8)	107(10)	83(8)	-4(7)	34(6)	38(7)
C62A	129(11)	97(13)	109(13)	-27(11)	2(9)	8(9)
C63A	164(16)	180(20)	120(16)	-75(15)	10(13)	-41(16)
O4B	137(9)	138(8)	128(8)	-76(6)	58(7)	4(6)
O5B	137(9)	138(8)	128(8)	-76(6)	58(7)	4(6)
C8B	57(7)	69(9)	30(8)	6(6)	9(6)	-2(6)
C9B	66(10)	74(9)	100(19)	24(9)	24(9)	-4(7)
C10B	80(9)	87(10)	54(15)	17(10)	22(8)	7(8)
C11B	79(10)	78(9)	67(14)	12(8)	25(8)	8(7)
C12B	73(8)	80(8)	35(9)	6(6)	18(7)	5(6)
C34B	48(6)	75(5)	50(5)	-25(4)	21(4)	-31(4)
C35B	51(6)	67(5)	50(6)	-16(4)	15(5)	-27(4)

Table S11 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for D2. 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}
C36B	76(8)	70(6)	91(8)	-9(5)	34(7)	-33(6)
C37B	132(15)	103(8)	107(10)	-17(7)	70(11)	-58(9)
C38B	180(20)	112(8)	108(11)	-29(7)	103(13)	-71(9)
C39B	119(13)	99(8)	75(7)	-31(6)	66(9)	-53(8)
C52B	30(7)	77(5)	55(6)	-47(4)	0(5)	-14(4)
C53B	39(6)	81(7)	64(7)	-50(6)	1(5)	-7(5)
C54B	48(8)	100(7)	81(8)	-53(6)	23(6)	-14(5)
C55B	27(6)	99(7)	52(7)	-47(5)	-4(5)	-18(5)
C56B	30(8)	99(10)	59(9)	-44(7)	4(7)	-20(8)
C57B	62(12)	101(10)	38(7)	-46(7)	5(7)	-29(8)
C58B	98(13)	102(10)	41(8)	-39(7)	27(8)	-25(9)
C59B	76(11)	99(8)	28(6)	-43(5)	6(6)	-27(7)
C60B	30(9)	96(7)	38(6)	-40(5)	-1(6)	-16(6)
C61B	137(9)	138(8)	128(8)	-76(6)	58(7)	4(6)
C62B	137(9)	138(8)	128(8)	-76(6)	58(7)	4(6)
C63B	137(9)	138(8)	128(8)	-76(6)	58(7)	4(6)
F1	350(13)	97(5)	183(8)	-8(5)	-80(8)	28(6)
F2	293(12)	130(6)	124(6)	22(5)	-42(6)	-57(7)
F3	222(8)	89(4)	123(5)	-20(4)	-42(5)	39(4)
F4	288(9)	120(6)	98(5)	-14(4)	-33(6)	-25(6)
B1	260(12)	80(7)	112(8)	11(6)	-48(8)	-2(7)

Table S12 Bond Lengths for D2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	P1	2.2664(17)	C45	C46	1.432(9)
Cu1	P2	2.2839(18)	C46	C47	1.377(11)
Cu1	N1	2.085(5)	C46	C49	1.505(11)
Cu1	N2	2.087(5)	C47	C48	1.404(11)
P1	C1	1.831(7)	C48	C52A	1.483(13)
P1	C7	1.826(9)	C48	C52B	1.484(14)
P1	C13	1.837(6)	C50	C51	1.508(10)
P2	C23	1.840(6)	O4A	C61A	1.071(18)
P2	C28	1.837(7)	O5A	C61A	1.36(3)
P2	C34A	2.06(3)	O5A	C62A	1.69(2)
P2	C34B	1.761(11)	C8A	C9A	1.39(2)
O1	C18	1.405(7)	C9A	C10A	1.41(3)
O1	C24	1.374(8)	C10A	C11A	1.43(3)
O2	C49	1.192(9)	C11A	C12A	1.41(2)
O3	C49	1.329(9)	C34A	C35A	1.38(4)
O3	C50	1.461(9)	C34A	C39A	1.42(3)

Table S12 Bond Lengths for D2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C40	1.381(7)	C35A	C36A	1.41(4)
N1	C48	1.330(8)	C36A	C37A	1.37(4)
N2	C52A	1.345(13)	C37A	C38A	1.38(4)
N2	C60A	1.374(12)	C38A	C39A	1.33(4)
N2	C52B	1.310(15)	C52A	C53A	1.429(14)
N2	C60B	1.407(13)	C53A	C54A	1.349(17)
C1	C2	1.359(12)	C54A	C55A	1.410(18)
C1	C6	1.379(10)	C54A	C61A	1.548(17)
C2	C3	1.388(12)	C55A	C56A	1.392(15)
C3	C4	1.381(14)	C55A	C60A	1.414(14)
C4	C5	1.293(16)	C56A	C57A	1.342(19)
C5	C6	1.396(15)	C57A	C58A	1.415(16)
C7	C8A	1.549(15)	C58A	C59A	1.354(13)
C7	C12A	1.235(18)	C59A	C60A	1.403(17)
C7	C8B	1.44(2)	C62A	C63A	1.60(3)
C7	C12B	1.46(2)	O4B	C61B	1.09(2)
C13	C14	1.408(10)	O5B	C61B	1.68(3)
C13	C18	1.397(9)	O5B	C62B	1.74(2)
C14	C15	1.390(9)	C8B	C9B	1.37(3)
C15	C16	1.378(11)	C9B	C10B	1.43(4)
C16	C17	1.399(9)	C10B	C11B	1.28(4)
C17	C18	1.385(8)	C11B	C12B	1.42(4)
C17	C25	1.539(10)	C34B	C35B	1.385(15)
C19	C20	1.360(11)	C34B	C39B	1.414(13)
C19	C24	1.402(8)	C35B	C36B	1.376(16)
C19	C25	1.527(10)	C36B	C37B	1.394(18)
C20	C21	1.402(12)	C37B	C38B	1.39(2)
C21	C22	1.403(9)	C38B	C39B	1.393(19)
C22	C23	1.397(10)	C52B	C53B	1.419(15)
C23	C24	1.397(9)	C53B	C54B	1.381(18)
C25	C26	1.537(11)	C54B	C55B	1.41(2)
C25	C27	1.531(9)	C54B	C61B	1.530(19)
C28	C29	1.368(11)	C55B	C56B	1.403(17)
C28	C33	1.352(12)	C55B	C60B	1.423(16)
C29	C30	1.434(15)	C56B	C57B	1.35(2)
C30	C31	1.278(18)	C57B	C58B	1.417(19)
C31	C32	1.377(16)	C58B	C59B	1.361(16)
C32	C33	1.402(11)	C59B	C60B	1.404(19)
C40	C41	1.417(8)	C62B	C63B	1.64(3)
C40	C45	1.413(9)	F1	B1	1.31(2)
C41	C42	1.364(8)	F2	B1	1.33(2)
C42	C43	1.398(9)	F3	B1	1.52(2)
C43	C44	1.372(9)	F4	B1	1.52(3)

Table S12 Bond Lengths for D2.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C44	C45	1.419(9)			

Table S13 Bond Angles for D2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P1	Cu1	P2	116.74(8)	C40	C45	C46	117.3(6)
N1	Cu1	P1	114.45(14)	C44	C45	C46	124.0(6)
N1	Cu1	P2	111.63(14)	C45	C46	C49	121.8(7)
N1	Cu1	N2	79.7(2)	C47	C46	C45	118.1(7)
N2	Cu1	P1	119.49(15)	C47	C46	C49	120.0(6)
N2	Cu1	P2	109.25(14)	C46	C47	C48	121.5(6)
C1	P1	Cu1	113.7(3)	N1	C48	C47	121.5(6)
C1	P1	C13	102.3(3)	N1	C48	C52A	115.0(8)
C7	P1	Cu1	116.2(3)	N1	C48	C52B	117.9(8)
C7	P1	C1	106.7(4)	C47	C48	C52A	123.0(7)
C7	P1	C13	102.0(4)	C47	C48	C52B	119.8(8)
C13	P1	Cu1	114.4(2)	O2	C49	O3	125.5(7)
C23	P2	Cu1	111.7(2)	O2	C49	C46	124.3(7)
C23	P2	C34A	106.6(7)	O3	C49	C46	110.3(6)
C28	P2	Cu1	116.5(2)	O3	C50	C51	106.1(6)
C28	P2	C23	105.0(3)	C61A	O5A	C62A	118.3(16)
C28	P2	C34A	114.5(7)	C9A	C8A	C7	118.1(15)
C34A	P2	Cu1	102.4(7)	C8A	C9A	C10A	118.6(14)
C34B	P2	Cu1	121.0(5)	C9A	C10A	C11A	120.7(16)
C34B	P2	C23	102.6(4)	C12A	C11A	C10A	117(2)
C34B	P2	C28	97.9(5)	C7	C12A	C11A	125.2(15)
C24	O1	C18	114.6(4)	C35A	C34A	P2	126.1(19)
C49	O3	C50	115.7(6)	C35A	C34A	C39A	113(3)
C40	N1	Cu1	128.9(4)	C39A	C34A	P2	120.5(19)
C48	N1	Cu1	112.3(4)	C34A	C35A	C36A	125(3)
C48	N1	C40	118.7(6)	C37A	C36A	C35A	118(3)
C52A	N2	Cu1	109.9(6)	C36A	C37A	C38A	120(3)
C52A	N2	C60A	112.5(8)	C39A	C38A	C37A	121(3)
C60A	N2	Cu1	130.3(10)	C38A	C39A	C34A	124(3)
C52B	N2	Cu1	114.4(6)	N2	C52A	C48	113.5(9)
C52B	N2	C60B	123.3(11)	N2	C52A	C53A	127.5(11)
C60B	N2	Cu1	122.2(10)	C53A	C52A	C48	118.9(11)
C2	C1	P1	117.9(5)	C54A	C53A	C52A	116.7(13)
C2	C1	C6	116.1(8)	C53A	C54A	C55A	120.1(11)
C6	C1	P1	125.9(8)	C53A	C54A	C61A	115.6(14)
C1	C2	C3	122.4(8)	C55A	C54A	C61A	124.1(12)
C4	C3	C2	118.8(11)	C54A	C55A	C60A	117.4(10)

Table S13 Bond Angles for D2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C5	C4	C3	120.1(10)	C56A	C55A	C54A	124.2(12)
C4	C5	C6	121.3(10)	C56A	C55A	C60A	118.4(13)
C1	C6	C5	121.2(11)	C57A	C56A	C55A	119.6(13)
C8A	C7	P1	113.0(9)	C56A	C57A	C58A	121.6(12)
C12A	C7	P1	127.4(8)	C59A	C58A	C57A	121.1(14)
C12A	C7	C8A	118.9(11)	C58A	C59A	C60A	117.2(12)
C8B	C7	P1	121.2(9)	N2	C60A	C55A	125.1(12)
C8B	C7	C12B	110.3(16)	N2	C60A	C59A	112.7(11)
C12B	C7	P1	119.7(10)	C59A	C60A	C55A	121.9(10)
C14	C13	P1	124.0(5)	O4A	C61A	O5A	113(2)
C18	C13	P1	118.7(5)	O4A	C61A	C54A	124.3(17)
C18	C13	C14	117.2(6)	O5A	C61A	C54A	105.8(16)
C15	C14	C13	119.2(7)	C63A	C62A	O5A	119.0(19)
C16	C15	C14	121.7(7)	C61B	O5B	C62B	134.6(16)
C15	C16	C17	120.9(6)	C9B	C8B	C7	124.6(19)
C16	C17	C25	125.1(5)	C8B	C9B	C10B	115(3)
C18	C17	C16	116.5(6)	C11B	C10B	C9B	126(3)
C18	C17	C25	118.4(6)	C10B	C11B	C12B	118(3)
C13	C18	O1	115.9(5)	C11B	C12B	C7	122(2)
C17	C18	O1	119.6(6)	C35B	C34B	P2	124.2(7)
C17	C18	C13	124.5(6)	C35B	C34B	C39B	118.9(10)
C20	C19	C24	116.8(7)	C39B	C34B	P2	116.6(9)
C20	C19	C25	125.6(6)	C36B	C35B	C34B	122.8(10)
C24	C19	C25	117.6(7)	C35B	C36B	C37B	117.5(13)
C19	C20	C21	122.3(6)	C38B	C37B	C36B	121.8(13)
C20	C21	C22	120.0(8)	C39B	C38B	C37B	119.6(12)
C23	C22	C21	119.1(7)	C38B	C39B	C34B	119.3(13)
C22	C23	P2	124.0(5)	N2	C52B	C48	115.5(10)
C22	C23	C24	118.3(5)	N2	C52B	C53B	117.0(11)
C24	C23	P2	117.5(5)	C53B	C52B	C48	124.9(12)
O1	C24	C19	120.5(6)	C54B	C53B	C52B	121.2(14)
O1	C24	C23	116.1(5)	C53B	C54B	C55B	122.0(12)
C23	C24	C19	123.4(7)	C53B	C54B	C61B	119.4(17)
C19	C25	C17	106.8(5)	C55B	C54B	C61B	118.3(16)
C19	C25	C26	109.4(6)	C54B	C55B	C60B	114.9(12)
C19	C25	C27	112.0(7)	C56B	C55B	C54B	123.4(13)
C26	C25	C17	108.9(7)	C56B	C55B	C60B	121.7(15)
C27	C25	C17	111.3(5)	C57B	C56B	C55B	117.8(15)
C27	C25	C26	108.3(6)	C56B	C57B	C58B	121.9(15)
C29	C28	P2	124.1(8)	C59B	C58B	C57B	119.7(17)
C33	C28	P2	119.8(5)	C58B	C59B	C60B	120.8(15)
C33	C28	C29	115.9(8)	N2	C60B	C55B	120.6(14)
C28	C29	C30	120.9(11)	C59B	C60B	N2	121.8(14)

Table S13 Bond Angles for D2.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C31	C30	C29	121.7(10)	C59B	C60B	C55B	117.3(12)
C30	C31	C32	119.4(10)	O4B	C61B	O5B	127.2(19)
C31	C32	C33	119.4(12)	O4B	C61B	C54B	131(2)
C28	C33	C32	122.7(9)	C54B	C61B	O5B	102.1(16)
N1	C40	C41	117.5(5)	C63B	C62B	O5B	85.4(18)
N1	C40	C45	122.8(5)	F1	B1	F2	117.6(16)
C45	C40	C41	119.6(5)	F1	B1	F3	108.6(18)
C42	C41	C40	120.2(6)	F1	B1	F4	108(2)
C41	C42	C43	120.4(5)	F2	B1	F3	113.1(19)
C44	C43	C42	120.9(6)	F2	B1	F4	104(2)
C43	C44	C45	120.2(6)	F3	B1	F4	104.4(13)
C40	C45	C44	118.6(5)				

Table S14 Torsion Angles for D2.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu1	P1	C1	C2	-27.2(6)	C29	C30	C31	C32	2.5(18)
Cu1	P1	C1	C6	148.5(6)	C30	C31	C32	C33	-1.9(15)
Cu1	P1	C7	C8A	-82.0(8)	C31	C32	C33	C28	-0.4(14)
Cu1	P1	C7	C12A	88.2(13)	C33	C28	C29	C30	-1.4(15)
Cu1	P1	C7	C8B	13.5(12)	C40	N1	C48	C47	-4.1(11)
Cu1	P1	C7	C12B	157.8(14)	C40	N1	C48	C52A	167.5(9)
Cu1	P1	C13	C14	132.2(6)	C40	N1	C48	C52B	-173.7(10)
Cu1	P1	C13	C18	-44.4(6)	C40	C41	C42	C43	2.2(9)
Cu1	P2	C23	C22	-125.0(6)	C40	C45	C46	C47	0.0(11)
Cu1	P2	C23	C24	49.8(6)	C40	C45	C46	C49	177.4(7)
Cu1	P2	C28	C29	-160.2(7)	C41	C40	C45	C44	-0.8(9)
Cu1	P2	C28	C33	15.2(7)	C41	C40	C45	C46	175.7(6)
Cu1	P2	C34B	C35B	-106.3(10)	C41	C42	C43	C44	-2.4(10)
Cu1	P2	C34B	C39B	66.4(12)	C42	C43	C44	C45	1.0(10)
Cu1	N1	C40	C41	9.3(8)	C43	C44	C45	C40	0.6(9)
Cu1	N1	C40	C45	-174.0(4)	C43	C44	C45	C46	-175.6(7)
Cu1	N1	C48	C47	173.4(7)	C44	C45	C46	C47	176.3(8)
Cu1	N1	C48	C52A	-15.0(11)	C44	C45	C46	C49	-6.3(11)
Cu1	N1	C48	C52B	3.8(11)	C45	C40	C41	C42	-0.6(9)
Cu1	N2	C52A	C48	-33.0(15)	C45	C46	C47	C48	-1.0(14)
Cu1	N2	C52A	C53A	149.9(16)	C45	C46	C49	O2	-35.5(13)
Cu1	N2	C60A	C55A	-146.0(19)	C45	C46	C49	O3	145.7(7)
Cu1	N2	C60A	C59A	41(3)	C46	C47	C48	N1	3.2(14)
Cu1	N2	C52B	C48	2.3(17)	C46	C47	C48	C52A	-167.7(12)
Cu1	N2	C52B	C53B	164.9(12)	C46	C47	C48	C52B	172.7(11)
Cu1	N2	C60B	C55B	-166(2)	C47	C46	C49	O2	141.9(10)

Table S14 Torsion Angles for D2.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu1	N2	C60B	C59B	8(4)	C47	C46	C49	O3	-37.0(12)
P1	C1	C2	C3	-179.1(6)	C47	C48	C52A	N2	-155.3(11)
P1	C1	C6	C5	-179.9(7)	C47	C48	C52A	C53A	22(2)
P1	C7	C8A	C9A	174.0(11)	C47	C48	C52B	N2	-174.0(11)
P1	C7	C12A	C11A	-166.5(17)	C47	C48	C52B	C53B	25(2)
P1	C7	C8B	C9B	172(2)	C48	N1	C40	C41	-173.7(6)
P1	C7	C12B	C11B	-170(2)	C48	N1	C40	C45	3.1(9)
P1	C13	C14	C15	-176.7(7)	C48	C52A	C53A	C54A	-176.7(16)
P1	C13	C18	O1	-3.4(8)	C48	C52B	C53B	C54B	168.7(16)
P1	C13	C18	C17	175.0(5)	C49	O3	C50	C51	178.7(8)
P2	C23	C24	O1	2.1(8)	C49	C46	C47	C48	-178.5(8)
P2	C23	C24	C19	-177.3(5)	C50	O3	C49	O2	-8.5(13)
P2	C28	C29	C30	174.2(8)	C50	O3	C49	C46	170.3(7)
P2	C28	C33	C32	-173.8(7)	C8A	C7	C12A	C11A	3(3)
P2	C34A	C35A	C36A	-174(2)	C8A	C9A	C10A	C11A	-9(3)
P2	C34A	C39A	C38A	177(2)	C9A	C10A	C11A	C12A	14(3)
P2	C34B	C35B	C36B	173.1(11)	C10A	C11A	C12A	C7	-12(4)
P2	C34B	C39B	C38B	-170.7(16)	C12A	C7	C8A	C9A	2.9(19)
N1	C40	C41	C42	176.3(5)	C34A	P2	C23	C22	123.9(10)
N1	C40	C45	C44	-177.5(6)	C34A	P2	C23	C24	-61.2(9)
N1	C40	C45	C46	-1.0(9)	C34A	P2	C28	C29	-40.9(11)
N1	C48	C52A	N2	33.2(17)	C34A	P2	C28	C33	134.6(9)
N1	C48	C52A	C53A	-149.4(14)	C34A	C35A	C36A	C37A	-1(5)
N1	C48	C52B	N2	-4.2(19)	C35A	C34A	C39A	C38A	4(4)
N1	C48	C52B	C53B	-165.2(14)	C35A	C36A	C37A	C38A	3(4)
N2	C52A	C53A	C54A	0(3)	C36A	C37A	C38A	C39A	-1(4)
N2	C52B	C53B	C54B	8(3)	C37A	C38A	C39A	C34A	-3(4)
C1	P1	C7	C8A	45.9(8)	C39A	C34A	C35A	C36A	-2(4)
C1	P1	C7	C12A	-143.9(13)	C52A	N2	C60A	C55A	1(4)
C1	P1	C7	C8B	141.5(11)	C52A	N2	C60A	C59A	-172.8(19)
C1	P1	C7	C12B	-74.2(15)	C52A	C53A	C54A	C55A	6(3)
C1	P1	C13	C14	8.8(8)	C52A	C53A	C54A	C61A	-178.3(19)
C1	P1	C13	C18	-167.8(6)	C53A	C54A	C55A	C56A	172.8(18)
C1	C2	C3	C4	-2.3(12)	C53A	C54A	C55A	C60A	-9(3)
C2	C1	C6	C5	-4.1(12)	C53A	C54A	C61A	O4A	-174(3)
C2	C3	C4	C5	-1.2(13)	C53A	C54A	C61A	O5A	53(3)
C3	C4	C5	C6	1.8(16)	C54A	C55A	C56A	C57A	-179.2(18)
C4	C5	C6	C1	1.0(16)	C54A	C55A	C60A	N2	5(4)
C6	C1	C2	C3	4.7(11)	C54A	C55A	C60A	C59A	178(2)
C7	P1	C1	C2	-156.6(6)	C55A	C54A	C61A	O4A	1(4)
C7	P1	C1	C6	19.1(7)	C55A	C54A	C61A	O5A	-132(2)
C7	P1	C13	C14	-101.4(7)	C55A	C56A	C57A	C58A	-3(3)
C7	P1	C13	C18	82.0(6)	C56A	C55A	C60A	N2	-176(2)

Table S14 Torsion Angles for D2.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C7	C8A	C9A	C10A	0(2)	C56A	C55A	C60A	C59A	-3(4)
C7	C8B	C9B	C10B	-16(5)	C56A	C57A	C58A	C59A	5(3)
C13	P1	C1	C2	96.7(6)	C57A	C58A	C59A	C60A	-5(3)
C13	P1	C1	C6	-87.6(7)	C58A	C59A	C60A	N2	178.4(19)
C13	P1	C7	C8A	152.8(7)	C58A	C59A	C60A	C55A	5(4)
C13	P1	C7	C12A	-37.0(13)	C60A	N2	C52A	C48	173.5(19)
C13	P1	C7	C8B	-111.7(12)	C60A	N2	C52A	C53A	-4(3)
C13	P1	C7	C12B	32.7(15)	C60A	C55A	C56A	C57A	2(3)
C13	C14	C15	C16	0.9(14)	C61A	O5A	C62A	C63A	-44(4)
C14	C13	C18	O1	179.7(6)	C61A	C54A	C55A	C56A	-2(3)
C14	C13	C18	C17	-1.8(11)	C61A	C54A	C55A	C60A	176(2)
C14	C15	C16	C17	0.0(13)	C62A	O5A	C61A	O4A	26(4)
C15	C16	C17	C18	-1.7(11)	C62A	O5A	C61A	C54A	165(2)
C15	C16	C17	C25	-179.9(7)	C8B	C7	C12B	C11B	-22(3)
C16	C17	C18	O1	-178.9(6)	C8B	C9B	C10B	C11B	3(6)
C16	C17	C18	C13	2.7(10)	C9B	C10B	C11B	C12B	-1(6)
C16	C17	C25	C19	-145.9(7)	C10B	C11B	C12B	C7	12(4)
C16	C17	C25	C26	96.1(8)	C12B	C7	C8B	C9B	25(3)
C16	C17	C25	C27	-23.3(10)	C34B	P2	C23	C22	104.0(8)
C18	O1	C24	C19	35.1(8)	C34B	P2	C23	C24	-81.2(7)
C18	O1	C24	C23	-144.3(6)	C34B	P2	C28	C29	-29.7(9)
C18	C13	C14	C15	0.0(12)	C34B	P2	C28	C33	145.8(7)
C18	C17	C25	C19	36.0(8)	C34B	C35B	C36B	C37B	-2(2)
C18	C17	C25	C26	-82.0(7)	C35B	C34B	C39B	C38B	2(2)
C18	C17	C25	C27	158.6(6)	C35B	C36B	C37B	C38B	0(3)
C19	C20	C21	C22	-2.3(14)	C36B	C37B	C38B	C39B	3(3)
C20	C19	C24	O1	-177.5(7)	C37B	C38B	C39B	C34B	-4(3)
C20	C19	C24	C23	1.9(11)	C39B	C34B	C35B	C36B	1(2)
C20	C19	C25	C17	144.1(8)	C52B	N2	C60B	C55B	11(4)
C20	C19	C25	C26	-98.1(9)	C52B	N2	C60B	C59B	-175(2)
C20	C19	C25	C27	22.0(10)	C52B	C53B	C54B	C55B	-3(3)
C20	C21	C22	C23	2.0(13)	C52B	C53B	C54B	C61B	170(2)
C21	C22	C23	P2	175.0(7)	C53B	C54B	C55B	C56B	-176.7(18)
C21	C22	C23	C24	0.2(11)	C53B	C54B	C55B	C60B	1(3)
C22	C23	C24	O1	177.3(6)	C53B	C54B	C61B	O4B	-144(4)
C22	C23	C24	C19	-2.2(10)	C53B	C54B	C61B	O5B	36(3)
C23	P2	C28	C29	75.7(8)	C54B	C55B	C56B	C57B	-175(2)
C23	P2	C28	C33	-108.9(6)	C54B	C55B	C60B	N2	-5(4)
C23	P2	C34B	C35B	18.9(12)	C54B	C55B	C60B	C59B	-179(2)
C23	P2	C34B	C39B	-168.4(11)	C55B	C54B	C61B	O4B	29(5)
C24	O1	C18	C13	141.5(6)	C55B	C54B	C61B	O5B	-151(2)
C24	O1	C18	C17	-37.0(8)	C55B	C56B	C57B	C58B	-6(3)
C24	C19	C20	C21	0.4(12)	C56B	C55B	C60B	N2	173(2)

Table S14 Torsion Angles for D2.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C24	C19	C25	C17	-37.8(8)	C56B	C55B	C60B	C59B	-1(4)
C24	C19	C25	C26	80.0(8)	C56B	C57B	C58B	C59B	-1(4)
C24	C19	C25	C27	-159.9(6)	C57B	C58B	C59B	C60B	7(4)
C25	C17	C18	O1	-0.6(9)	C58B	C59B	C60B	N2	180(3)
C25	C17	C18	C13	-179.0(6)	C58B	C59B	C60B	C55B	-6(4)
C25	C19	C20	C21	178.5(8)	C60B	N2	C52B	C48	-175(2)
C25	C19	C24	O1	4.2(9)	C60B	N2	C52B	C53B	-12(3)
C25	C19	C24	C23	-176.4(6)	C60B	C55B	C56B	C57B	7(3)
C28	P2	C23	C22	2.1(7)	C61B	O5B	C62B	C63B	-135(3)
C28	P2	C23	C24	176.9(5)	C61B	C54B	C55B	C56B	10(3)
C28	P2	C34B	C35B	126.2(11)	C61B	C54B	C55B	C60B	-172(3)
C28	P2	C34B	C39B	-61.1(11)	C62B	O5B	C61B	O4B	11(6)
C28	C29	C30	C31	-0.9(19)	C62B	O5B	C61B	C54B	-169(3)
C29	C28	C33	C32	2.0(13)					

Table S15 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for D2.

Atom	*x*	*y*	*z*	U(eq)
H2	3410.92	4772.22	3023.58	88
H3	4623.22	5466.34	3533.66	104
H4	6086.49	4430.49	4520.15	112
H5	6277.8	2804.2	4982.41	130
H6	5101.71	2089.94	4465.96	104
H14	5935.84	2466.51	2811.97	89
H15	7130.01	1916.13	1834.39	87
H16	6228.85	1555.42	906.83	71
H20	2066.17	2684.09	-480.64	91
H21	3.49	3814.08	-540.09	104
H22	-978.61	4149.38	574.36	82
H26A	4572.18	89.07	1095.21	135
H26B	3238.72	432.23	662.46	135
H26C	3285.01	503.71	1510.47	135
H27A	4449.5	2415.51	-240.66	102
H27B	3985.55	1562.92	-388.85	102
H27C	5300.82	1251.77	55.38	102
H29	-2527.26	3507.8	1835.24	138
H30	-4596.4	4700.97	1650.04	137
H31	-4973.08	6274.92	1688.74	132
H32	-3281.23	6805.58	1822.27	120
H33	-1221.58	5650.22	1984.49	92
H41	2649.7	4132.56	1309.4	52

Table S15 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for D2.

Atom	*x*	*y*	*z*	U(eq)
H42	3685.5	4362.19	180.64	57
H43	3943.09	5917.73	-408.91	63
H44	3037.76	7285.69	77.04	63
H47	494.1	7703.03	2184.54	100
H50A	900.88	10346.39	356.7	89
H50B	1231.89	10181.55	1230.12	89
H51A	-1283.33	10690.5	661.47	120
H51B	-749.04	11498.26	825.24	120
H51C	-921.58	10601.95	1509.72	120
H8A	2795.3	2408.99	4793.99	104
H9A	2445.04	1038	5710.64	126
H10A	2659.18	-439.4	5357.4	125
H11A	2623.62	-347.2	4036.97	150
H12A	3311.65	901.39	3202.92	113
H35A	739.41	1239.21	2300.3	58
H36A	649.05	-244.13	3176.19	80
H37A	18.13	-182.49	4403.28	78
H38A	-666.64	1358.83	4689.75	70
H39A	-680.47	2781.52	3820.49	65
H53A	-1372.88	7481.31	2597.63	97
H56A	-3026.12	5924.08	4800.17	80
H57A	-2274.22	4366.24	5645.13	73
H58A	-500.93	3099.52	5384.18	68
H59A	727.31	3473.17	4355.68	59
H62A	-5281.63	9307.61	2728.54	149
H62B	-5589.48	8666.45	2243.9	149
H63A	-6811.9	8092.96	3141.63	226
H63B	-6772.01	8951.49	3508.27	226
H63C	-5799.51	7826.85	3804.98	226
H8B	1215.88	1990.48	3674.09	74
H9B	1064.48	500.44	4491.69	116
H10B	2999.24	-872.41	4808.59	110
H11B	4878.65	-723.44	4541.15	110
H12B	4997.8	839.85	3774.57	91
H35B	523.46	1526.92	2050.83	66
H36B	129.09	95.89	2793.48	97
H37B	-1017.93	202.33	3898.42	138
H38B	-1727.23	1699.12	4258.22	157
H39B	-1470.44	3171.63	3444.81	114
H53B	-858.2	7433.53	3069.6	70
H56B	-2649.14	5636.09	5085.45	70
H57B	-2105.94	3940.95	5701.41	74

Table S15 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for D2.

Atom	*x*	*y*	*z*	U(eq)
H58B	-565.51	2720.93	5222.46	96
H59B	386.18	3217.75	4099.38	76
H62C	-4036.66	9726.45	3863.71	170
H62D	-3082.37	9999	3190.35	170
H63D	-5127.29	10088.55	2578.78	213
H63E	-3950.07	9206.72	2394.03	213
H63F	-4882.97	8940.27	3052.3	213

Table S16 Atomic Occupancy for D2.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
O4A	0.551(9)	O5A	0.551(9)	C8A	0.655(10)
H8A	0.655(10)	C9A	0.655(10)	H9A	0.655(10)
C10A	0.655(10)	H10A	0.655(10)	C11A	0.655(10)
H11A	0.655(10)	C12A	0.655(10)	H12A	0.655(10)
C34A	0.278(18)	C35A	0.278(18)	H35A	0.278(18)
C36A	0.278(18)	H36A	0.278(18)	C37A	0.278(18)
H37A	0.278(18)	C38A	0.278(18)	H38A	0.278(18)
C39A	0.278(18)	H39A	0.278(18)	C52A	0.551(9)
C53A	0.551(9)	H53A	0.551(9)	C54A	0.551(9)
C55A	0.551(9)	C56A	0.551(9)	H56A	0.551(9)
C57A	0.551(9)	H57A	0.551(9)	C58A	0.551(9)
H58A	0.551(9)	C59A	0.551(9)	H59A	0.551(9)
C60A	0.551(9)	C61A	0.551(9)	C62A	0.551(9)
H62A	0.551(9)	H62B	0.551(9)	C63A	0.551(9)
H63A	0.551(9)	H63B	0.551(9)	H63C	0.551(9)
O4B	0.449(9)	O5B	0.449(9)	C8B	0.345(10)
H8B	0.345(10)	C9B	0.345(10)	H9B	0.345(10)
C10B	0.345(10)	H10B	0.345(10)	C11B	0.345(10)
H11B	0.345(10)	C12B	0.345(10)	H12B	0.345(10)
C34B	0.722(18)	C35B	0.722(18)	H35B	0.722(18)
C36B	0.722(18)	H36B	0.722(18)	C37B	0.722(18)
H37B	0.722(18)	C38B	0.722(18)	H38B	0.722(18)
C39B	0.722(18)	H39B	0.722(18)	C52B	0.449(9)
C53B	0.449(9)	H53B	0.449(9)	C54B	0.449(9)
C55B	0.449(9)	C56B	0.449(9)	H56B	0.449(9)
C57B	0.449(9)	H57B	0.449(9)	C58B	0.449(9)
H58B	0.449(9)	C59B	0.449(9)	H59B	0.449(9)
C60B	0.449(9)	C61B	0.449(9)	C62B	0.449(9)
H62C	0.449(9)	H62D	0.449(9)	C63B	0.449(9)
H63D	0.449(9)	H63E	0.449(9)	H63F	0.449(9)

Crystal structure determination of D2

Crystal Data for $C_{63}H_{52}BCuF_4N_2O_5P_2$ (M =1129.35 g/mol): triclinic, space group P-1 (no. 2), a = 11.2410(5) Å, b = 14.6532(8) Å, c = 18.4225(8) Å, α = 73.672(3)°, β = 86.086(3)°, γ = 70.147(3)°, V = 2737.8(2) Å^3, Z = 2, T = 100.00 K, μ(CuKα) = 1.668 mm^{-1}, *Dcalc* = 1.370 g/cm^3, 57710 reflections measured (5° ≤ 2Θ ≤ 141.634°), 10363 unique (R_{int} = 0.1112, R_{sigma} = 0.0731) which were used in all calculations. The final R_1 was 0.0962 (I > 2σ(I)) and wR_2 was 0.3004 (all data).

6. Crystallography data for complex **D3**

Table S17 Crystal data and structure refinement for D3.

Identification code	**D3**
Empirical formula	$C_{60}H_{48}BCuF_4N_2O_5P_2$
Formula weight	1089.29
Temperature/K	100
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	17.2437(18)
b/Å	10.7278(10)
c/Å	29.075(3)
α/°	90
β/°	103.722(5)
γ/°	90
Volume/Å^3	5224.9(9)
Z	4
ρ_{calc}g/cm^3	1.385
μ/mm^{-1}	0.546
F(000)	2248.0
Crystal size/mm^3	0.43 × 0.14 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.906 to 55.308
Index ranges	-22 ≤ h ≤ 22, -13 ≤ k ≤ 13, -37 ≤ l ≤ 37
Reflections collected	45782
Independent reflections	11928 [R_{int} = 0.1572, R_{sigma} = 0.2010]
Data/restraints/parameters	11928/762/802
Goodness-of-fit on F^2	1.023
Final R indexes [I>=2σ (I)]	R_1 = 0.0931, wR_2 = 0.2018
Final R indexes [all data]	R_1 = 0.2138, wR_2 = 0.2538
Largest diff. peak/hole / e Å^{-3}	0.98/-0.83

Table S18 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for D3. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Cu1	4314.4(5)	5500.4(7)	6901.6(3)	28.5(2)

Table S18 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for D3. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
P1	3152.7(10)	5755.8(15)	6372.5(5)	27.3(4)
P2	5429.4(10)	5129.2(15)	6604.1(5)	25.5(4)
O2	6958(3)	9481(6)	8484(2)	75.4(19)
O5	5115(5)	3090(6)	9183.8(19)	90(2)
O3	6223(3)	8629(5)	8936.2(16)	49.2(13)
O4	5541(5)	1392(7)	8862(2)	93(2)
N1	4834(3)	6807(5)	7419.7(17)	28.7(11)
N2	4534(3)	4406(5)	7499.9(17)	31.7(12)
C59	5431(10)	2542(12)	9666(3)	141(6)
C48	4955(5)	3096(7)	8361(2)	47.5(18)
C57	6394(6)	8903(10)	9759(3)	82(3)
C34	7339(5)	4851(7)	8022(2)	48.4(18)
C53	3975(4)	2558(6)	7091(2)	38.8(16)
C36	6373(4)	3881(6)	7379(2)	36.1(15)
C46	4912(4)	4984(6)	7900(2)	32.6(14)
C38	4788(4)	8453(6)	6858(2)	38.1(16)
C50	4312(5)	1177(7)	7935(3)	48.6(18)
C40	5629(5)	10243(7)	7078(3)	52.2(19)
C55	6409(4)	8838(7)	8535(3)	43.8(17)
C42	5612(4)	8688(6)	7671(2)	37.4(15)
C44	5616(4)	6989(7)	8216(2)	35.9(15)
C33	7215(4)	5962(7)	7781(2)	41.6(17)
C7A	5188(4)	7053(6)	5935(2)	33.4(14)
C35	6913(4)	3795(7)	7821(2)	45.8(18)
C8A	5394(5)	7978(7)	5656(2)	49.7(18)
C37	5075(4)	7979(6)	7322(2)	31.9(14)
C9A	6192(6)	8182(7)	5685(3)	58(2)
C39	5067(5)	9563(7)	6736(3)	47.2(18)
C10A	6780(5)	7456(7)	5977(3)	55(2)
C41	5877(5)	9853(7)	7521(3)	49.6(18)
C11A	6547(4)	6526(6)	6246(2)	39.6(16)
C43	5857(4)	8157(7)	8135(2)	37.4(15)
C12A	5745(4)	6306(6)	6237(2)	30.5(14)
C45	5117(4)	6310(6)	7848(2)	32.1(14)
C12B	5501(4)	3702(6)	6275(2)	32.8(14)
C47	5130(5)	4351(7)	8339(2)	45.8(18)
C7B	4804(5)	3106(6)	6026(2)	38.4(15)
C49	4562(4)	2452(7)	7949(2)	39.5(16)
C8B	4850(6)	2046(7)	5753(2)	53.0(19)
C52	3742(5)	1337(7)	7091(3)	47.5(19)
C9B	5578(6)	1575(7)	5738(3)	64(2)

Table S18 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for D3. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C54	4363(4)	3149(6)	7519(2)	33.5(14)
C10B	6271(6)	2144(8)	5985(3)	71(2)
C56	6735(5)	9195(8)	9354(3)	62(2)
C11B	6231(5)	3188(7)	6257(2)	49.2(19)
C58	5234(7)	2409(10)	8827(3)	74(3)
C31	6253(4)	4998(6)	7130.5(19)	27.5(13)
C60	5351(11)	3383(14)	10010(4)	168(7)
C32	6677(4)	6054(6)	7343(2)	33.7(15)
C51	3917(5)	649(7)	7523(3)	48.8(18)
O1B	3980(9)	3925(13)	5960(4)	32(3)
C16B	1255(17)	2730(30)	6226(9)	47(6)
C15B	1460(30)	3330(40)	6590(14)	39(8)
C14B	2070(20)	4290(40)	6652(13)	46(10)
C17B	1580(20)	2880(30)	5860(10)	74(10)
C19B	2568(10)	7163(14)	6412(6)	28(5)
C20B	1932(10)	7581(15)	6057(5)	44(5)
C21B	1526(8)	8661(15)	6124(5)	54(7)
C22B	1757(9)	9322(13)	6546(6)	40(5)
C23B	2394(10)	8904(17)	6900(5)	53(8)
C24B	2800(9)	7825(18)	6833(5)	35(6)
C13B	2410(20)	4590(30)	6298(11)	38(6)
C18B	2159(17)	3800(30)	5890(9)	58(8)
C6B	3814(9)	4883(11)	5649(4)	27(4)
C5B	4064(9)	4902(12)	5228(5)	28(5)
C4B	3892(9)	5925(14)	4927(4)	41(6)
C3B	3469(9)	6928(11)	5048(4)	33(5)
C2B	3220(8)	6909(11)	5468(4)	26(4)
C1B	3392(8)	5886(13)	5769(4)	22(4)
F1	2624(8)	-837(12)	4728(4)	228(5)
F4	2047(6)	952(9)	4595(5)	203(4)
F2	1236(6)	-674(7)	4459(4)	177(4)
F3	2078(6)	-473(11)	4055(3)	201(4)
B1	1996(13)	-209(18)	4484(7)	118(4)
O1A	4323(3)	6863(5)	5920.0(18)	26.3(13)
C16A	917(8)	3340(11)	6361(4)	50(3)
C15A	1615(10)	3180(19)	6731(5)	47(3)
C13A	2249(8)	4838(12)	6397(4)	30(3)
C17A	886(6)	4258(10)	6036(4)	43(2)
C19A	2740(4)	7329(5)	6320(2)	27(2)
C20A	2594(4)	8012(6)	5901.6(19)	39(2)
C21A	2231(4)	9174(5)	5879(2)	47(3)

Table S18 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for D3. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C22A	2013(4)	9653(5)	6275(3)	48(3)
C23A	2159(5)	8970(7)	6693(2)	48(3)
C24A	2523(5)	7808(6)	6715(2)	40(3)
C1A	3321(3)	5298(5)	5790.6(15)	24.9(19)
C6A	3918(3)	5920(4)	5634.8(17)	23.4(17)
C5A	4116(3)	5550(5)	5218.7(18)	29(2)
C4A	3716(3)	4558(5)	4958.5(15)	32(2)
C3A	3119(3)	3936(4)	5114.4(17)	34(2)
C2A	2921(3)	4306(5)	5530.4(18)	28.5(19)
C18A	1532(5)	5034(9)	6051(3)	37(2)
C14A	2279(9)	3930(13)	6748(5)	37(3)

Table S19 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for D3. 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}
Cu1	28.9(4)	31.3(5)	23.6(4)	-4.0(3)	2.7(3)	0.5(4)
P1	25.6(9)	32.7(10)	22.9(8)	-2.9(6)	4.1(6)	-1.1(7)
P2	27.9(9)	25.6(10)	21.7(8)	-1.1(6)	3.5(6)	2.2(7)
O2	53(4)	105(5)	67(4)	-31(3)	12(3)	-35(3)
O5	165(7)	68(4)	33(3)	9(3)	19(3)	-19(4)
O3	41(3)	65(4)	34(2)	-14(2)	-7(2)	-9(2)
O4	135(6)	66(4)	62(4)	22(3)	-9(4)	8(4)
N1	30(3)	29(3)	27(2)	-7.6(19)	8(2)	0(2)
N2	34(3)	35(3)	26(2)	-2(2)	7(2)	-4(2)
C59	262(16)	112(9)	33(4)	19(4)	6(6)	-42(9)
C48	63(5)	46(4)	34(3)	6(3)	12(3)	-4(3)
C57	86(7)	111(8)	41(4)	-28(4)	-4(4)	-36(6)
C34	46(4)	64(4)	31(3)	0(3)	0(3)	12(3)
C53	45(4)	40(4)	34(3)	-3(3)	14(3)	-10(3)
C36	41(4)	36(4)	31(3)	8(3)	7(3)	11(3)
C46	34(4)	38(3)	26(3)	-4(2)	8(2)	-2(3)
C38	47(4)	33(4)	35(3)	-6(2)	12(3)	10(3)
C50	66(5)	36(4)	48(4)	4(3)	23(3)	1(3)
C40	69(5)	36(4)	57(4)	-11(3)	27(3)	-9(3)
C55	31(4)	51(4)	44(3)	-16(3)	-3(3)	0(3)
C42	30(4)	37(3)	45(3)	-15(2)	10(3)	-1(3)
C44	28(3)	46(4)	31(3)	-13(3)	2(3)	1(3)
C33	33(4)	54(4)	33(3)	-10(3)	-1(3)	4(3)
C7A	45(3)	26(3)	27(3)	-1(2)	5(2)	5(2)
C35	49(4)	53(4)	32(3)	10(3)	2(3)	12(3)

Table S19 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for D3. 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}
C8A	79(5)	33(4)	35(4)	3(3)	8(3)	-4(3)
C37	32(3)	32(3)	33(3)	-8(2)	9(2)	0(2)
C9A	87(5)	41(5)	46(4)	8(3)	17(4)	-10(4)
C39	69(5)	31(4)	46(4)	-7(3)	22(3)	-2(3)
C10A	61(5)	54(5)	50(4)	4(3)	14(3)	-19(3)
C41	55(5)	40(4)	56(4)	-21(3)	16(3)	-13(3)
C11A	45(4)	38(4)	36(4)	4(3)	10(3)	-6(3)
C43	26(3)	44(4)	40(3)	-16(2)	3(3)	2(3)
C12A	43(3)	23(3)	24(3)	-2(2)	6(2)	-2(2)
C45	31(3)	38(3)	25(3)	-6(2)	4(2)	-1(2)
C12B	50(4)	30(3)	18(3)	1(2)	9(2)	2(3)
C47	59(5)	50(4)	25(3)	0(3)	3(3)	-5(3)
C7B	57(4)	34(4)	23(3)	-2(2)	6(3)	-3(3)
C49	49(4)	41(3)	35(3)	3(2)	21(3)	2(3)
C8B	95(5)	33(4)	25(3)	-4(3)	2(3)	-3(3)
C52	67(5)	38(4)	43(4)	-3(3)	25(3)	-15(3)
C9B	116(6)	31(4)	40(4)	-6(3)	8(4)	22(4)
C54	34(4)	37(3)	34(3)	-1(2)	17(3)	-2(3)
C10B	100(6)	56(5)	55(5)	-13(4)	13(4)	32(4)
C56	52(5)	80(6)	40(4)	-24(4)	-15(3)	-13(4)
C11B	63(4)	48(4)	37(4)	-5(3)	13(3)	20(3)
C58	113(7)	65(5)	37(4)	15(3)	5(4)	-9(4)
C31	28(3)	34(3)	18(3)	2(2)	2(2)	4(2)
C60	290(20)	155(12)	61(6)	-11(7)	46(9)	-92(12)
C32	30(3)	39(4)	30(3)	-5(2)	5(3)	8(3)
C51	68(5)	39(4)	48(4)	1(3)	31(3)	-4(3)
O1B	54(6)	25(6)	13(6)	-3(4)	-1(5)	-1(5)
C16B	54(13)	45(13)	45(10)	-3(9)	17(9)	-11(11)
C15B	45(15)	35(13)	37(11)	7(9)	11(10)	2(12)
C14B	56(17)	48(17)	37(10)	-3(9)	19(10)	-11(15)
C17B	91(18)	87(16)	51(11)	-21(11)	31(11)	-48(16)
C19B	18(8)	34(8)	37(8)	2(5)	15(6)	-15(6)
C20B	34(9)	51(10)	44(9)	-3(7)	6(7)	-6(7)
C21B	42(11)	55(11)	60(10)	-7(8)	1(8)	3(9)
C22B	20(10)	44(10)	56(10)	-1(8)	7(8)	-9(8)
C23B	38(12)	59(12)	55(11)	-20(9)	-5(9)	11(10)
C24B	17(10)	45(10)	44(9)	-4(7)	9(7)	-4(7)
C13B	41(11)	44(10)	30(9)	1(6)	9(7)	-8(8)
C18B	72(15)	68(13)	38(9)	-9(9)	21(9)	-28(12)
C6B	32(9)	31(7)	18(6)	0(5)	3(6)	3(6)
C5B	30(11)	37(10)	15(6)	1(6)	0(7)	10(8)
C4B	50(14)	47(9)	28(8)	11(7)	10(8)	17(9)

Table S19 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for D3. 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}
C3B	31(11)	35(9)	33(8)	10(6)	6(7)	5(7)
C2B	16(9)	31(8)	28(7)	7(5)	-1(6)	3(6)
C1B	18(8)	25(7)	21(6)	-1(4)	-2(5)	-1(6)
F1	248(10)	280(11)	155(8)	-18(7)	45(7)	117(9)
F4	171(8)	128(6)	358(13)	-43(7)	155(8)	-11(5)
F2	173(7)	99(6)	310(11)	-32(6)	159(7)	-2(5)
F3	161(8)	316(12)	137(6)	-31(7)	59(6)	27(8)
B1	144(9)	104(8)	128(8)	10(7)	78(7)	7(6)
O1A	33(3)	21(3)	22(3)	-2(2)	3(2)	3(2)
C16A	52(6)	57(6)	49(5)	-15(4)	26(5)	-11(5)
C15A	48(6)	59(7)	42(7)	-10(5)	28(5)	-9(5)
C13A	34(5)	28(5)	31(5)	-8(4)	12(3)	-4(4)
C17A	35(5)	54(6)	42(5)	-14(4)	13(4)	-16(4)
C19A	14(5)	31(4)	34(4)	-7(3)	1(3)	-3(3)
C20A	41(6)	36(5)	37(4)	-10(3)	2(4)	2(4)
C21A	49(6)	33(5)	53(5)	-7(4)	3(4)	7(4)
C22A	40(6)	39(6)	62(5)	-16(4)	5(4)	-2(4)
C23A	37(7)	42(5)	65(6)	-18(4)	10(5)	-3(5)
C24A	35(7)	45(5)	42(5)	-13(4)	10(4)	-3(5)
C1A	29(4)	22(4)	20(4)	2(3)	-1(3)	4(3)
C6A	28(4)	20(4)	18(3)	2(3)	-3(3)	9(3)
C5A	35(5)	28(5)	21(4)	-1(3)	1(3)	6(4)
C4A	37(5)	34(5)	22(4)	-7(3)	2(3)	7(4)
C3A	36(5)	36(5)	24(4)	-6(3)	-2(3)	3(4)
C2A	30(4)	29(5)	24(4)	-3(3)	2(3)	2(3)
C18A	31(4)	50(5)	33(4)	-4(4)	11(3)	-8(4)
C14A	39(6)	43(7)	32(5)	1(4)	17(4)	0(5)

Table S20 Bond Lengths for D3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	P1	2.2344(18)	C10A	C11A	1.384(9)
Cu1	P2	2.3222(18)	C11A	C12A	1.398(9)
Cu1	N1	2.097(5)	C12B	C7B	1.401(9)
Cu1	N2	2.058(5)	C12B	C11B	1.387(9)
P1	C19B	1.834(12)	C7B	C8B	1.400(9)
P1	C13B	1.77(3)	C7B	O1B	1.642(16)
P1	C1B	1.901(9)	C49	C54	1.427(9)
P1	C13A	1.859(13)	C8B	C9B	1.364(12)
P1	C19A	1.824(5)	C52	C51	1.424(10)
P1	C1A	1.849(4)	C9B	C10B	1.382(13)

Table S20 Bond Lengths for D3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P2	C12A	1.818(6)	C10B	C11B	1.382(10)
P2	C12B	1.825(6)	C31	C32	1.409(9)
P2	C31	1.830(6)	O1B	C6B	1.355(16)
O2	C55	1.208(9)	C16B	C15B	1.22(5)
O5	C59	1.499(11)	C16B	C17B	1.32(3)
O5	C58	1.325(11)	C15B	C14B	1.45(5)
O3	C55	1.301(9)	C14B	C13B	1.34(5)
O3	C56	1.455(8)	C17B	C18B	1.39(4)
O4	C58	1.206(11)	C19B	C20B	1.3900
N1	C37	1.374(8)	C19B	C24B	1.3900
N1	C45	1.335(8)	C20B	C21B	1.3900
N2	C46	1.343(8)	C21B	C22B	1.3900
N2	C54	1.384(8)	C22B	C23B	1.3900
C59	C60	1.378(17)	C23B	C24B	1.3900
C48	C47	1.385(10)	C13B	C18B	1.44(4)
C48	C49	1.410(10)	C6B	C5B	1.3900
C48	C58	1.516(11)	C6B	C1B	1.3900
C57	C56	1.469(12)	C5B	C4B	1.3900
C34	C33	1.373(10)	C4B	C3B	1.3900
C34	C35	1.400(11)	C3B	C2B	1.3900
C53	C52	1.371(9)	C2B	C1B	1.3900
C53	C54	1.414(9)	F1	B1	1.33(2)
C36	C35	1.399(9)	F4	B1	1.285(19)
C36	C31	1.390(9)	F2	B1	1.39(2)
C46	C45	1.483(9)	F3	B1	1.318(18)
C46	C47	1.416(9)	O1A	C6A	1.387(7)
C38	C37	1.417(9)	C16A	C15A	1.42(2)
C38	C39	1.363(10)	C16A	C17A	1.356(15)
C50	C49	1.431(10)	C15A	C14A	1.390(19)
C50	C51	1.353(10)	C13A	C18A	1.412(16)
C40	C39	1.415(10)	C13A	C14A	1.404(18)
C40	C41	1.326(11)	C17A	C18A	1.383(13)
C55	C43	1.506(9)	C19A	C20A	1.3900
C42	C37	1.422(9)	C19A	C24A	1.3900
C42	C41	1.434(10)	C20A	C21A	1.3900
C42	C43	1.432(9)	C21A	C22A	1.3900
C44	C43	1.357(10)	C22A	C23A	1.3900
C44	C45	1.407(8)	C23A	C24A	1.3900
C33	C32	1.390(9)	C1A	C6A	1.3900
C7A	C8A	1.381(9)	C1A	C2A	1.3900
C7A	C12A	1.389(9)	C6A	C5A	1.3900
C7A	O1A	1.497(9)	C5A	C4A	1.3900
C8A	C9A	1.376(11)	C4A	C3A	1.3900

Table S20 Bond Lengths for D3.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C9A	C10A	1.396(11)	C3A	C2A	1.3900

Table S21 Bond Angles for D3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
P1	Cu1	P2	116.80(6)	C8B	C7B	O1B	122.1(8)
N1	Cu1	P1	124.95(15)	C48	C49	C50	125.0(6)
N1	Cu1	P2	97.59(14)	C48	C49	C54	117.1(6)
N2	Cu1	P1	127.37(15)	C54	C49	C50	117.9(7)
N2	Cu1	P2	102.40(15)	C9B	C8B	C7B	119.7(8)
N2	Cu1	N1	79.2(2)	C53	C52	C51	119.6(7)
C19B	P1	Cu1	118.3(6)	C8B	C9B	C10B	120.6(8)
C19B	P1	C1B	103.8(7)	N2	C54	C53	117.5(6)
C13B	P1	Cu1	120.3(12)	N2	C54	C49	122.4(6)
C13B	P1	C19B	101.2(13)	C53	C54	C49	120.0(6)
C13B	P1	C1B	104.5(11)	C9B	C10B	C11B	120.0(9)
C1B	P1	Cu1	106.8(4)	O3	C56	C57	107.5(7)
C13A	P1	Cu1	122.1(4)	C10B	C11B	C12B	120.8(8)
C19A	P1	Cu1	116.1(2)	O5	C58	C48	110.9(9)
C19A	P1	C13A	100.3(5)	O4	C58	O5	125.2(8)
C19A	P1	C1A	108.1(3)	O4	C58	C48	123.8(9)
C1A	P1	Cu1	106.71(19)	C36	C31	P2	119.5(5)
C1A	P1	C13A	102.1(4)	C36	C31	C32	117.9(6)
C12A	P2	Cu1	119.3(2)	C32	C31	P2	121.6(5)
C12A	P2	C12B	102.0(3)	C33	C32	C31	120.6(6)
C12A	P2	C31	105.3(3)	C50	C51	C52	121.3(7)
C12B	P2	Cu1	120.3(2)	C6B	O1B	C7B	121.6(12)
C12B	P2	C31	103.8(3)	C15B	C16B	C17B	123(3)
C31	P2	Cu1	104.4(2)	C16B	C15B	C14B	122(4)
C58	O5	C59	115.4(9)	C13B	C14B	C15B	121(4)
C55	O3	C56	116.5(6)	C16B	C17B	C18B	118(3)
C37	N1	Cu1	124.2(4)	C20B	C19B	P1	124.7(10)
C45	N1	Cu1	113.7(4)	C20B	C19B	C24B	120.0
C45	N1	C37	119.7(5)	C24B	C19B	P1	115.3(10)
C46	N2	Cu1	115.1(4)	C19B	C20B	C21B	120.0
C46	N2	C54	118.6(5)	C22B	C21B	C20B	120.0
C54	N2	Cu1	126.2(4)	C21B	C22B	C23B	120.0
C60	C59	O5	110.3(12)	C22B	C23B	C24B	120.0
C47	C48	C49	120.3(6)	C23B	C24B	C19B	120.0
C47	C48	C58	119.2(7)	C14B	C13B	P1	121(3)
C49	C48	C58	120.5(7)	C14B	C13B	C18B	113(3)
C33	C34	C35	119.1(7)	C18B	C13B	P1	126(2)

Table S21 Bond Angles for D3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C52	C53	C54	120.4(7)	C17B	C18B	C13B	123(3)
C31	C36	C35	121.3(7)	O1B	C6B	C5B	122.6(11)
N2	C46	C45	115.6(5)	O1B	C6B	C1B	117.4(11)
N2	C46	C47	122.1(6)	C5B	C6B	C1B	120.0
C47	C46	C45	122.3(6)	C4B	C5B	C6B	120.0
C39	C38	C37	119.8(7)	C3B	C4B	C5B	120.0
C51	C50	C49	120.7(7)	C2B	C3B	C4B	120.0
C41	C40	C39	122.0(7)	C3B	C2B	C1B	120.0
O2	C55	O3	125.1(7)	C6B	C1B	P1	114.6(7)
O2	C55	C43	123.6(7)	C2B	C1B	P1	125.3(7)
O3	C55	C43	111.3(7)	C2B	C1B	C6B	120.0
C37	C42	C41	116.7(6)	F1	B1	F2	119.0(16)
C37	C42	C43	117.1(6)	F4	B1	F1	111.0(19)
C43	C42	C41	126.1(6)	F4	B1	F2	111.6(16)
C43	C44	C45	120.2(6)	F4	B1	F3	115.5(15)
C34	C33	C32	121.2(7)	F3	B1	F1	98.1(15)
C8A	C7A	C12A	123.4(7)	F3	B1	F2	100.7(16)
C8A	C7A	O1A	118.2(6)	C6A	O1A	C7A	118.3(5)
C12A	C7A	O1A	118.4(6)	C17A	C16A	C15A	120.1(13)
C36	C35	C34	119.9(7)	C14A	C15A	C16A	119.9(15)
C9A	C8A	C7A	118.1(7)	C18A	C13A	P1	119.6(9)
N1	C37	C38	118.0(6)	C14A	C13A	P1	120.6(10)
N1	C37	C42	121.3(6)	C14A	C13A	C18A	119.8(12)
C38	C37	C42	120.6(6)	C16A	C17A	C18A	121.1(11)
C8A	C9A	C10A	121.4(7)	C20A	C19A	P1	123.2(4)
C38	C39	C40	119.5(7)	C20A	C19A	C24A	120.0
C11A	C10A	C9A	118.6(8)	C24A	C19A	P1	116.7(4)
C40	C41	C42	121.2(7)	C19A	C20A	C21A	120.0
C10A	C11A	C12A	122.0(7)	C22A	C21A	C20A	120.0
C42	C43	C55	121.6(7)	C21A	C22A	C23A	120.0
C44	C43	C55	118.6(6)	C24A	C23A	C22A	120.0
C44	C43	C42	119.7(6)	C23A	C24A	C19A	120.0
C7A	C12A	P2	120.8(5)	C6A	C1A	P1	117.4(3)
C7A	C12A	C11A	116.5(6)	C6A	C1A	C2A	120.0
C11A	C12A	P2	122.6(5)	C2A	C1A	P1	122.4(3)
N1	C45	C46	115.8(5)	O1A	C6A	C1A	117.5(4)
N1	C45	C44	121.7(6)	O1A	C6A	C5A	122.4(4)
C44	C45	C46	122.4(6)	C1A	C6A	C5A	120.0
C7B	C12B	P2	119.8(5)	C6A	C5A	C4A	120.0
C11B	C12B	P2	121.8(5)	C3A	C4A	C5A	120.0
C11B	C12B	C7B	118.4(6)	C2A	C3A	C4A	120.0
C48	C47	C46	119.5(6)	C3A	C2A	C1A	120.0
C12B	C7B	O1B	115.4(7)	C17A	C18A	C13A	119.7(10)

Table S21 Bond Angles for D3.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C8B	C7B	C12B	120.4(7)	C15A	C14A	C13A	119.2(13)

Table S22 Torsion Angles for D3.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Cu1	P1	C19B	C20B	165.7(9)	C12B	C7B	O1B	C6B	74.5(13)
Cu1	P1	C19B	C24B	-14.5(10)	C47	C48	C49	C50	-176.4(7)
Cu1	P1	C13B	C14B	63(4)	C47	C48	C49	C54	0.2(11)
Cu1	P1	C13B	C18B	-110(3)	C47	C48	C58	O5	42.9(12)
Cu1	P1	C13A	C18A	-179.6(6)	C47	C48	C58	O4	-135.3(10)
Cu1	P1	C13A	C14A	-1.3(12)	C47	C46	C45	N1	-176.3(6)
Cu1	P1	C19A	C20A	119.7(4)	C47	C46	C45	C44	7.1(10)
Cu1	P1	C19A	C24A	-64.3(4)	C7B	C12B	C11B	C10B	2.7(11)
Cu1	P1	C1A	C6A	-57.1(3)	C7B	C8B	C9B	C10B	-0.8(12)
Cu1	P1	C1A	C2A	117.6(3)	C7B	O1B	C6B	C5B	31.6(17)
Cu1	P2	C12A	C7A	-33.6(6)	C7B	O1B	C6B	C1B	-146.9(9)
Cu1	P2	C12A	C11A	145.2(5)	C49	C48	C47	C46	0.1(11)
Cu1	P2	C12B	C7B	27.5(6)	C49	C48	C58	O5	-140.7(8)
Cu1	P2	C12B	C11B	-153.3(5)	C49	C48	C58	O4	41.1(14)
Cu1	P2	C31	C36	80.8(5)	C49	C50	C51	C52	0.5(12)
Cu1	P2	C31	C32	-87.1(5)	C8B	C7B	O1B	C6B	-89.2(14)
Cu1	N1	C37	C38	16.1(8)	C8B	C9B	C10B	C11B	1.2(13)
Cu1	N1	C37	C42	-162.4(5)	C52	C53	C54	N2	-175.7(6)
Cu1	N1	C45	C46	-8.9(7)	C52	C53	C54	C49	4.2(10)
Cu1	N1	C45	C44	167.8(5)	C9B	C10B	C11B	C12B	-2.1(12)
Cu1	N2	C46	C45	-0.6(7)	C54	N2	C46	C45	176.5(5)
Cu1	N2	C46	C47	-177.8(5)	C54	N2	C46	C47	-0.8(9)
Cu1	N2	C54	C53	-2.4(8)	C54	C53	C52	C51	-2.2(11)
Cu1	N2	C54	C49	177.8(5)	C56	O3	C55	O2	-1.6(12)
P1	C19B	C20B	C21B	179.7(13)	C56	O3	C55	C43	177.5(6)
P1	C19B	C24B	C23B	-179.7(12)	C11B	C12B	C7B	C8B	-2.4(9)
P1	C13B	C18B	C17B	178(3)	C11B	C12B	C7B	O1B	-166.4(7)
P1	C13A	C18A	C17A	172.7(7)	C58	O5	C59	C60	173.6(12)
P1	C13A	C14A	C15A	-174.0(11)	C58	C48	C47	C46	176.5(8)
P1	C19A	C20A	C21A	175.8(5)	C58	C48	C49	C50	7.3(12)
P1	C19A	C24A	C23A	-176.1(5)	C58	C48	C49	C54	-176.2(7)
P1	C1A	C6A	O1A	-2.1(5)	C31	P2	C12A	C7A	-150.3(5)
P1	C1A	C6A	C5A	174.9(4)	C31	P2	C12A	C11A	28.6(6)
P1	C1A	C2A	C3A	-174.6(4)	C31	P2	C12B	C7B	143.6(5)
P2	C12B	C7B	C8B	176.8(5)	C31	P2	C12B	C11B	-37.2(6)
P2	C12B	C7B	O1B	12.8(9)	C31	C36	C35	C34	0.6(10)
P2	C12B	C11B	C10B	-176.5(6)	C51	C50	C49	C48	178.0(8)

Table S22 Torsion Angles for D3.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
P2	C31	C32	C33	170.0(5)	C51	C50	C49	C54	1.5(11)
O2	C55	C43	C42	-36.8(11)	O1B	C7B	C8B	C9B	164.4(8)
O2	C55	C43	C44	140.5(8)	O1B	C6B	C5B	C4B	-178.4(15)
O3	C55	C43	C42	144.1(6)	O1B	C6B	C1B	P1	2.2(13)
O3	C55	C43	C44	-38.7(9)	O1B	C6B	C1B	C2B	178.5(14)
N2	C46	C45	N1	6.4(8)	C16B	C15B	C14B	C13B	4(6)
N2	C46	C45	C44	-170.2(6)	C16B	C17B	C18B	C13B	-1(5)
N2	C46	C47	C48	0.2(11)	C15B	C16B	C17B	C18B	-2(6)
C59	O5	C58	O4	2.9(16)	C15B	C14B	C13B	P1	180(3)
C59	O5	C58	C48	-175.3(9)	C15B	C14B	C13B	C18B	-6(5)
C48	C49	C54	N2	-0.8(10)	C14B	C13B	C18B	C17B	5(5)
C48	C49	C54	C53	179.4(7)	C17B	C16B	C15B	C14B	1(6)
C34	C33	C32	C31	-1.1(10)	C19B	P1	C13B	C14B	-70(3)
C53	C52	C51	C50	-0.2(12)	C19B	P1	C13B	C18B	117(3)
C36	C31	C32	C33	2.0(9)	C19B	C20B	C21B	C22B	0.0
C46	N2	C54	C53	-179.1(6)	C20B	C19B	C24B	C23B	0.0
C46	N2	C54	C49	1.0(9)	C20B	C21B	C22B	C23B	0.0
C50	C49	C54	N2	176.0(6)	C21B	C22B	C23B	C24B	0.0
C50	C49	C54	C53	-3.8(10)	C22B	C23B	C24B	C19B	0.0
C55	O3	C56	C57	176.8(7)	C24B	C19B	C20B	C21B	0.0
C33	C34	C35	C36	0.3(11)	C13B	P1	C19B	C20B	-60.5(15)
C7A	C8A	C9A	C10A	1.8(12)	C13B	P1	C19B	C24B	119.2(13)
C7A	O1A	C6A	C1A	146.0(5)	C6B	C5B	C4B	C3B	0.0
C7A	O1A	C6A	C5A	-31.0(7)	C5B	C6B	C1B	P1	-176.3(10)
C35	C34	C33	C32	-0.1(11)	C5B	C6B	C1B	C2B	0.0
C35	C36	C31	P2	-170.1(5)	C5B	C4B	C3B	C2B	0.0
C35	C36	C31	C32	-1.7(9)	C4B	C3B	C2B	C1B	0.0
C8A	C7A	C12A	P2	178.6(5)	C3B	C2B	C1B	P1	175.9(12)
C8A	C7A	C12A	C11A	-0.3(10)	C3B	C2B	C1B	C6B	0.0
C8A	C7A	O1A	C6A	98.2(7)	C1B	P1	C19B	C20B	47.6(12)
C8A	C9A	C10A	C11A	-0.8(12)	C1B	P1	C19B	C24B	-132.7(9)
C37	N1	C45	C46	-172.0(5)	C1B	P1	C13B	C14B	-177(3)
C37	N1	C45	C44	4.6(9)	C1B	P1	C13B	C18B	10(3)
C37	C38	C39	C40	-1.3(10)	C1B	C6B	C5B	C4B	0.0
C37	C42	C41	C40	0.0(11)	O1A	C7A	C8A	C9A	177.5(6)
C37	C42	C43	C55	-178.6(6)	O1A	C7A	C12A	P2	-0.2(8)
C37	C42	C43	C44	4.2(9)	O1A	C7A	C12A	C11A	-179.0(5)
C9A	C10A	C11A	C12A	-0.8(11)	O1A	C6A	C5A	C4A	176.9(6)
C39	C38	C37	N1	-174.3(6)	C16A	C15A	C14A	C13A	0(2)
C39	C38	C37	C42	4.1(10)	C16A	C17A	C18A	C13A	2.7(15)
C39	C40	C41	C42	2.8(12)	C15A	C16A	C17A	C18A	1.5(18)
C10A	C11A	C12A	P2	-177.6(6)	C13A	P1	C19A	C20A	-106.6(5)
C10A	C11A	C12A	C7A	1.3(10)	C13A	P1	C19A	C24A	69.4(5)

Table S22 Torsion Angles for D3.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C41	C40	C39	C38	-2.2(12)	C13A	P1	C1A	C6A	173.7(5)
C41	C42	C37	N1	174.9(6)	C13A	P1	C1A	C2A	-11.6(6)
C41	C42	C37	C38	-3.5(9)	C17A	C16A	C15A	C14A	-3(2)
C41	C42	C43	C55	3.5(11)	C19A	P1	C13A	C18A	50.5(8)
C41	C42	C43	C44	-173.8(7)	C19A	P1	C13A	C14A	-131.3(10)
C43	C42	C37	N1	-3.3(9)	C19A	P1	C1A	C6A	68.4(4)
C43	C42	C37	C38	178.3(6)	C19A	P1	C1A	C2A	-116.8(4)
C43	C42	C41	C40	178.0(7)	C19A	C20A	C21A	C22A	0.0
C43	C44	C45	N1	-3.6(10)	C20A	C19A	C24A	C23A	0.0
C43	C44	C45	C46	172.8(6)	C20A	C21A	C22A	C23A	0.0
C12A	P2	C12B	C7B	-107.1(5)	C21A	C22A	C23A	C24A	0.0
C12A	P2	C12B	C11B	72.1(6)	C22A	C23A	C24A	C19A	0.0
C12A	P2	C31	C36	-152.8(5)	C24A	C19A	C20A	C21A	0.0
C12A	P2	C31	C32	39.4(6)	C1A	P1	C13A	C18A	-60.8(9)
C12A	C7A	C8A	C9A	-1.2(11)	C1A	P1	C13A	C14A	117.5(10)
C12A	C7A	O1A	C6A	-82.9(7)	C1A	P1	C19A	C20A	-0.1(5)
C45	N1	C37	C38	177.3(6)	C1A	P1	C19A	C24A	175.9(4)
C45	N1	C37	C42	-1.1(9)	C1A	C6A	C5A	C4A	0.0
C45	C46	C47	C48	-176.9(7)	C6A	C1A	C2A	C3A	0.0
C45	C44	C43	C55	-178.3(6)	C6A	C5A	C4A	C3A	0.0
C45	C44	C43	C42	-1.0(10)	C5A	C4A	C3A	C2A	0.0
C12B	P2	C12A	C7A	101.6(5)	C4A	C3A	C2A	C1A	0.0
C12B	P2	C12A	C11A	-79.6(6)	C2A	C1A	C6A	O1A	-177.0(5)
C12B	P2	C31	C36	-46.0(6)	C2A	C1A	C6A	C5A	0.0
C12B	P2	C31	C32	146.2(5)	C18A	C13A	C14A	C15A	4(2)
C12B	C7B	C8B	C9B	1.4(10)	C14A	C13A	C18A	C17A	-5.6(16)

Table S23 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for D3.

Atom	*x*	*y*	*z*	U(eq)
H59A	5133.49	1770.48	9698.67	169
H59B	6000.76	2322.64	9707.35	169
H57A	5873.41	9311.76	9717.06	124
H57B	6753.31	9203.73	10051.48	124
H57C	6327.21	7999.05	9779.13	124
H34	7708.38	4799.44	8321.02	58
H53	3875.98	3010.34	6802.25	47
H36	6082.33	3161.71	7247.09	43
H38	4401.81	7998.38	6632.74	46
H50	4425.4	696.33	8217.08	58
H40	5835.4	11001.15	6986.67	63

Table S23 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for D3.

Atom	*x*	*y*	*z*	U(eq)
H44	5783.8	6630.05	8522.13	43
H33	7502.31	6680.77	7916.22	50
H7A	4638.5	6920.3	5921.2	40
H35	6990.26	3020.81	7984.68	55
H8A	4995.41	8459.17	5449.71	60
H9A	6345.14	8830.1	5502.1	69
H39	4885.62	9878.23	6423.27	57
H10A	7329.29	7598.05	5991.15	66
H41	6237.13	10355.5	7743.36	60
H11A	6944.62	6022.68	6442.3	48
H47	5395.61	4784.49	8617.09	55
H7B	4297.12	3424.25	6042.99	46
H8B	4375.64	1655.77	5579.46	64
H52	3466.04	950.48	6805.35	57
H9B	5608.93	848.56	5556.55	77
H10B	6775.61	1818.38	5967.61	85
H56A	6758.69	10109.3	9312.57	74
H56B	7283.37	8856.71	9407.62	74
H11B	6709.55	3557.8	6434.65	59
H60A	5620.96	4162.97	9967.12	252
H60B	5592.37	3036.77	10323.68	252
H60C	4783.58	3546.94	9985.43	252
H32	6594.35	6835.83	7185.53	40
H51	3752.87	-196.14	7521.4	59
H16B	845.78	2122.04	6204.13	57
H15B	1209.69	3172.65	6841.99	46
H14B	2235.6	4701.11	6947.89	55
H17B	1420.87	2371.02	5585.79	88
H20B	1773.78	7129.61	5768.93	53
H21B	1090.8	8946.17	5881.76	65
H22B	1479.78	10059.12	6591.37	48
H23B	2551.74	9355.53	7188.15	64
H24B	3234.72	7538.97	7075.33	42
H18B	2400.68	3901.59	5630.66	69
H5B	4352.26	4215.86	5145.65	34
H4B	4062.38	5937.81	4639.93	50
H3B	3351.79	7627.43	4842.39	40
H2B	2931.07	7595.12	5550.55	32
H16A	472.61	2802.55	6340.56	60
H15A	1628.05	2560.61	6966.43	56
H17A	412.26	4369.98	5794.51	52
H20A	2742.52	7684.08	5631.26	47

Table S23 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for D3.

Atom	*x*	*y*	*z*	U(eq)
H21A	2130.71	9640.61	5593.46	56
H22A	1764.82	10447.52	6259.37	58
H23A	2010.73	9297.91	6963.1	58
H24A	2622.54	7341.37	7000.91	48
H5A	4523.69	5974.9	5112.16	34
H4A	3850.69	4305.33	4674.12	38
H3A	2845.43	3258.48	4936.53	40
H2A	2513.16	3881.19	5636.97	34
H18A	1493.8	5695.78	5829.86	44
H14A	2747	3829.09	6995.07	44

Table S24 Atomic Occupancy for D3.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
H7A	0.293(4)	H7B	0.707(4)	O1B	0.293(4)
C16B	0.293(4)	H16B	0.293(4)	C15B	0.293(4)
H15B	0.293(4)	C14B	0.293(4)	H14B	0.293(4)
C17B	0.293(4)	H17B	0.293(4)	C19B	0.293(4)
C20B	0.293(4)	H20B	0.293(4)	C21B	0.293(4)
H21B	0.293(4)	C22B	0.293(4)	H22B	0.293(4)
C23B	0.293(4)	H23B	0.293(4)	C24B	0.293(4)
H24B	0.293(4)	C13B	0.293(4)	C18B	0.293(4)
H18B	0.293(4)	C6B	0.293(4)	C5B	0.293(4)
H5B	0.293(4)	C4B	0.293(4)	H4B	0.293(4)
C3B	0.293(4)	H3B	0.293(4)	C2B	0.293(4)
H2B	0.293(4)	C1B	0.293(4)	O1A	0.707(4)
C16A	0.707(4)	H16A	0.707(4)	C15A	0.707(4)
H15A	0.707(4)	C13A	0.707(4)	C17A	0.707(4)
H17A	0.707(4)	C19A	0.707(4)	C20A	0.707(4)
H20A	0.707(4)	C21A	0.707(4)	H21A	0.707(4)
C22A	0.707(4)	H22A	0.707(4)	C23A	0.707(4)
H23A	0.707(4)	C24A	0.707(4)	H24A	0.707(4)
C1A	0.707(4)	C6A	0.707(4)	C5A	0.707(4)
H5A	0.707(4)	C4A	0.707(4)	H4A	0.707(4)
C3A	0.707(4)	H3A	0.707(4)	C2A	0.707(4)
H2A	0.707(4)	C18A	0.707(4)	H18A	0.707(4)
C14A	0.707(4)	H14A	0.707(4)		

6.1. Crystal structure determination of D3

Crystal Data for $C_{60}H_{48}BCuF_4N_2O_5P_2$ (*M* =1089.29 g/mol): monoclinic, space group $P2_1/n$ (no. 14), *a* = 17.2437(18) Å, *b* = 10.7278(10) Å, *c* = 29.075(3) Å, *β* = 103.722(5)°, *V* = 5224.9(9) Å^3, *Z* = 4, *T* = 100 K, μ(MoKα) = 0.546 mm^{-1}, *Dcalc* = 1.385 g/cm^3, 45782 reflections measured (4.906° ≤ 2Θ ≤ 55.308°), 11928 unique

(R_{int} = 0.1572, R_{sigma} = 0.2010) which were used in all calculations. The final R_1 was 0.0931 (I > 2σ(I)) and wR_2 was 0.2538 (all data).

Table S25. Calculated bond lengths and angles

Complexes	**D2**	**D3**	**D1**
Bond Lengths (Å)			
Cu-N_1	1.99(1)	1.99(1)	2.04(7)
Cu-N_2	1.95(3)	1.95(3)	2.11(8)
Cu-P_1/Cu-N_3	2.46(3)	2.46(3)	2.04(2)
Cu-P2/Cu-N_4	2.48(5)	2.48(5)	2.09(8)
Cu-O_1	3.08(1)	3.08(1)	-
Dihedral angle			
N_1-Cu-N_2 to P_1-Cu-P_2/N_3-Cu-N_4	86.7(4)	93.3(5)	74.7(9)
Bond angles (˚)			
N_1-Cu-N_2	88.6(3)	88.63(3)	80.1(3)
P_1-Cu-P_2 / N_3-Cu-N_4	123.29(5)	123.29(5)	80.6(5)
P_1–Cu–N_1 /N_1-Cu-N_3	114.98(5)	114.98(5)	118.2(2)
P_1–Cu–N_2 /N_2-Cu-N_3	103.90(5)	103.90(5)	127.2(6)
P_2–Cu–N_1 /N_1-Cu-N_4	111.06(5)	111.06(5)	117.0(1)
P_2–Cu–N_2 /N_2-Cu-N_4	108.54(1)	108.54(1)	127.2(6)

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