

New unsymmetrical tetraazaphenathrene-based Cu(I) complexes: Synthesis, characterization, crystal structure and computational studies

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Supplementary Information

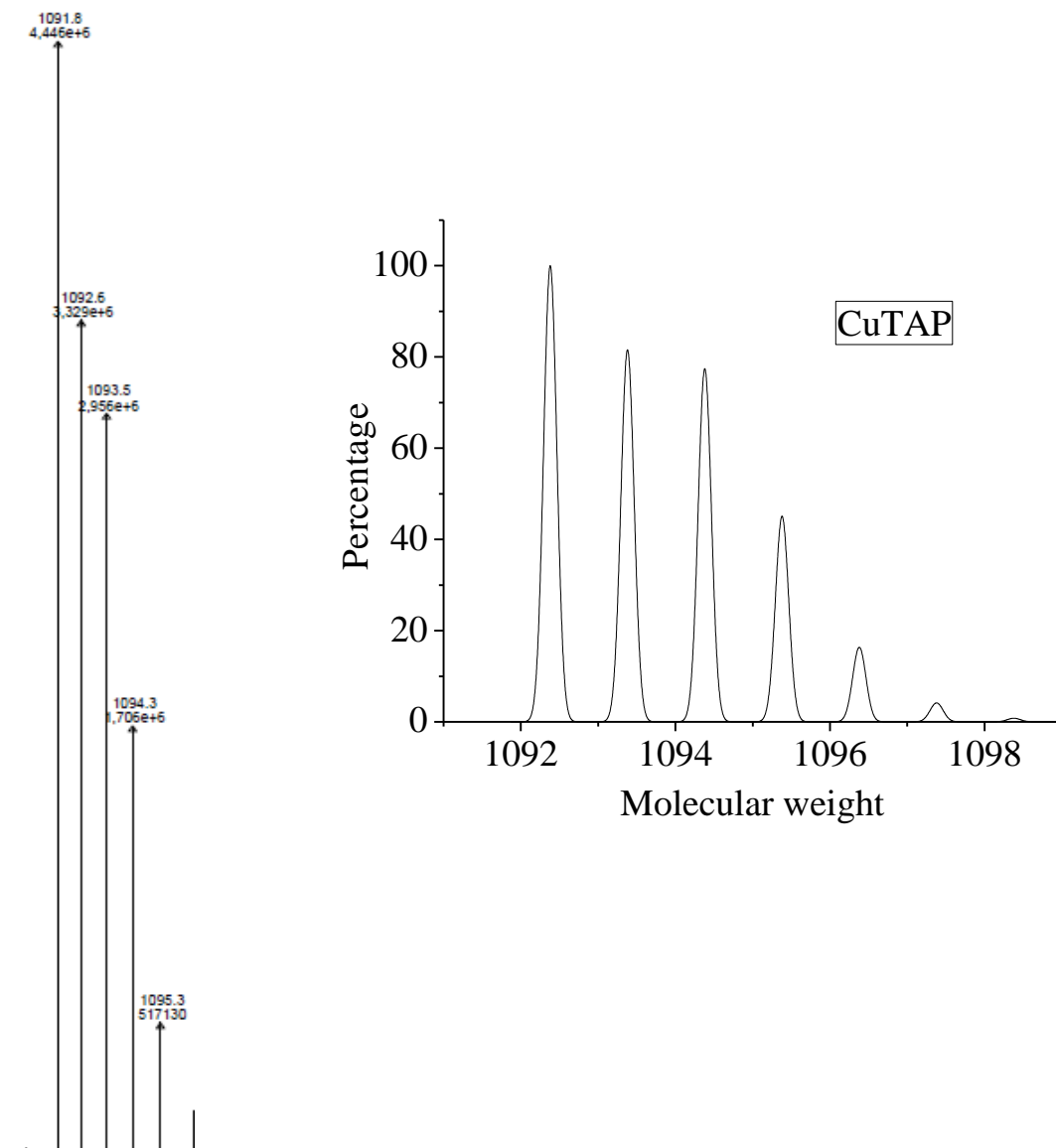


Fig. S1. Experimental ESI-MS (left) and the simulated spectrum (right) of complex **1**.

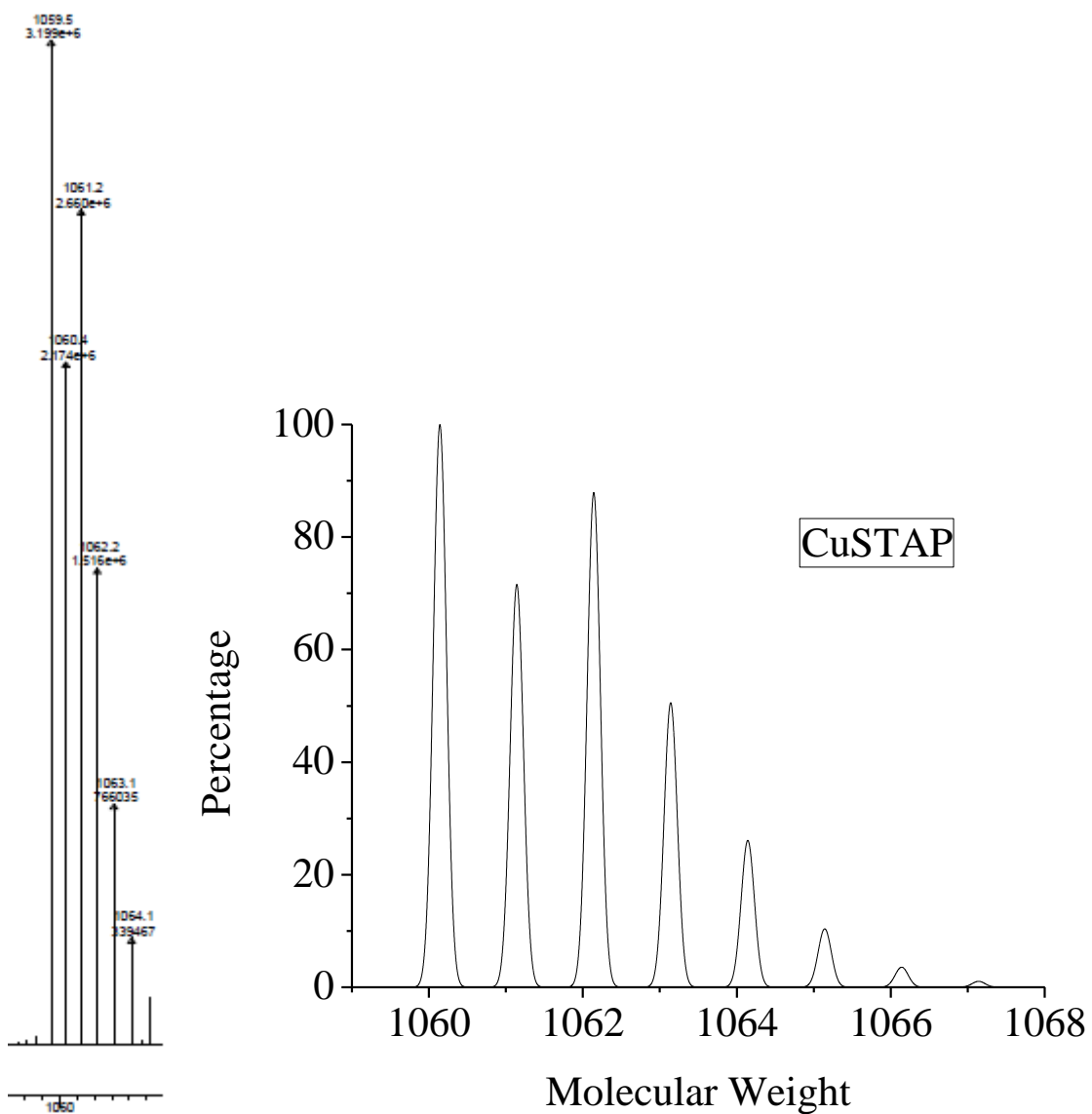


Fig. S2. Experimental ESI-MS and the simulated spectrum of complex 2.

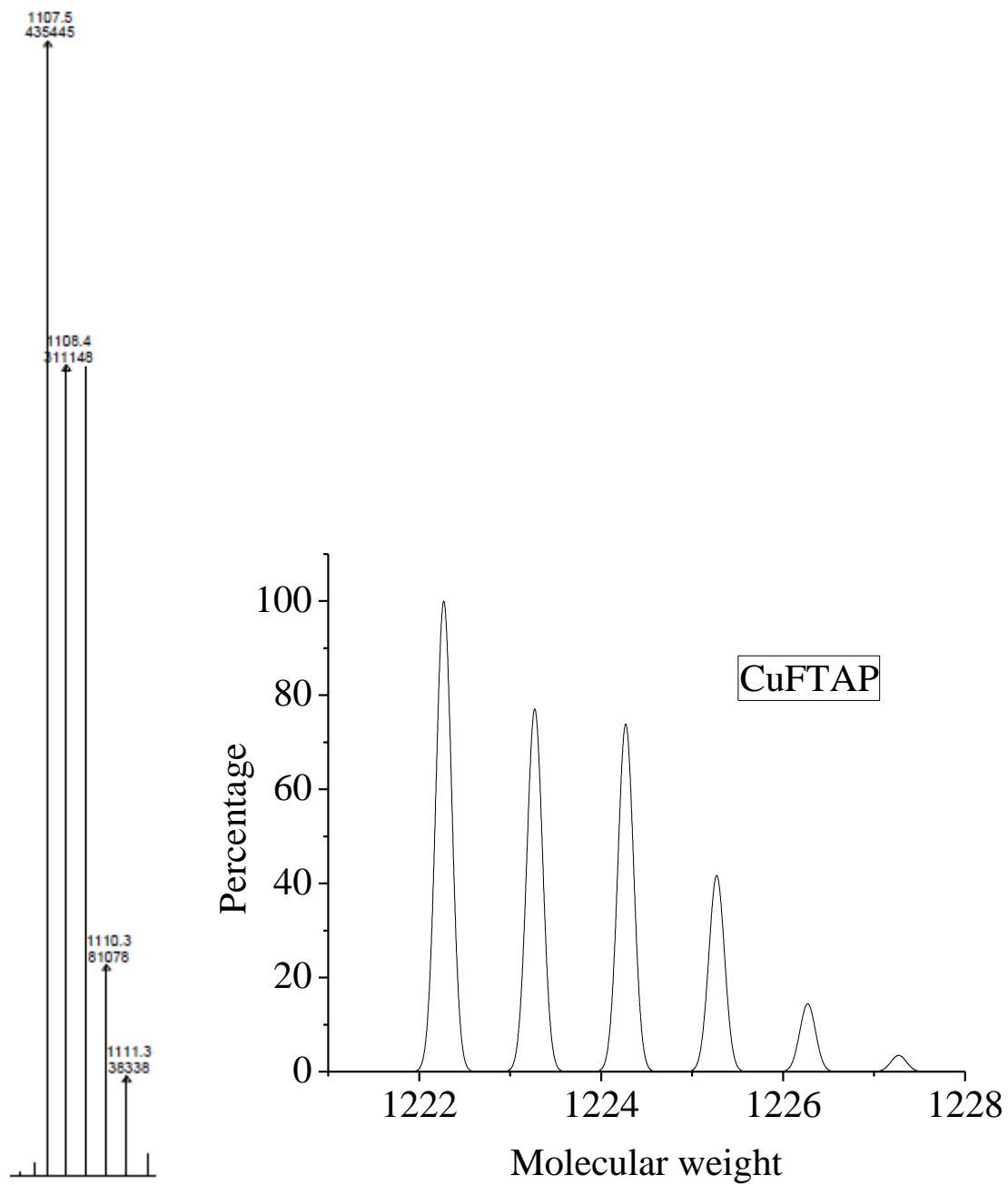


Fig. S3. Experimental ESI-MS (left) and the simulated spectrum (right) of complex 3.

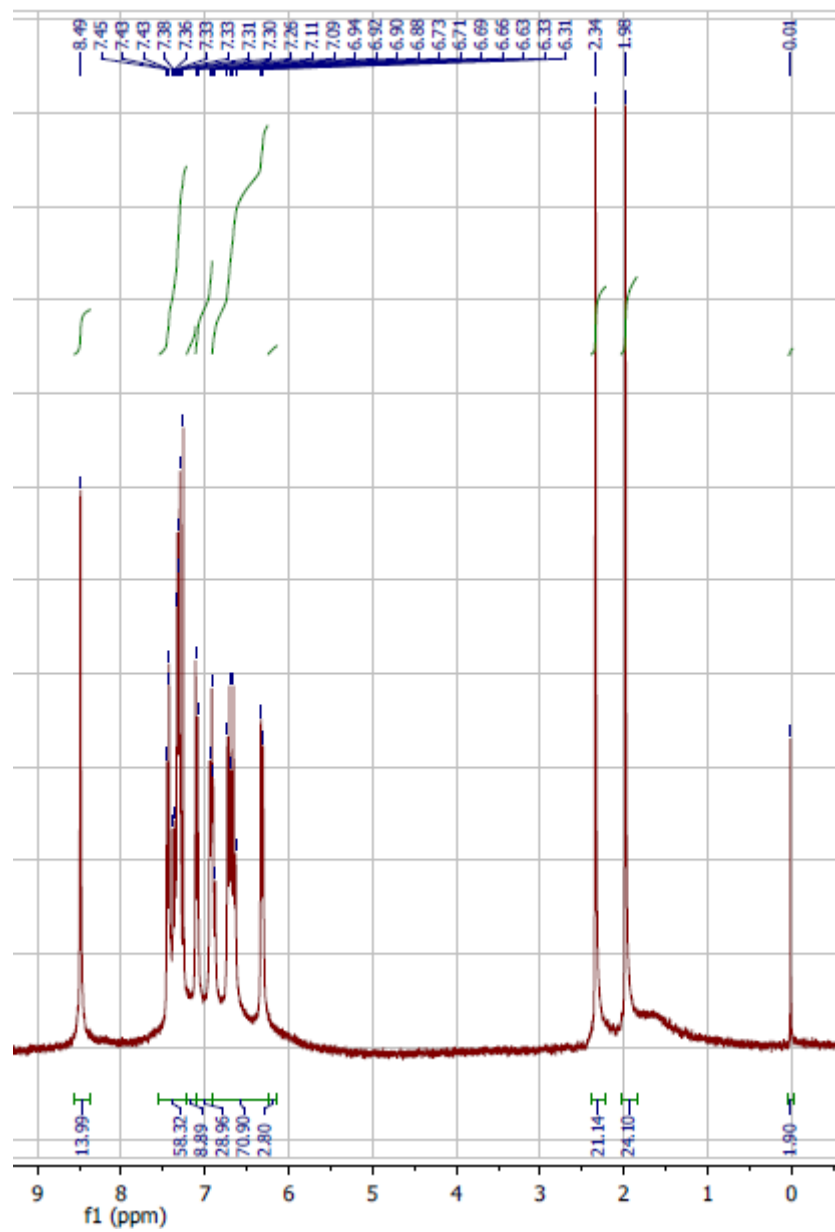


Fig. S4. $^1\text{H-NMR}$ spectrum of complex 1 in CDCl_3 .

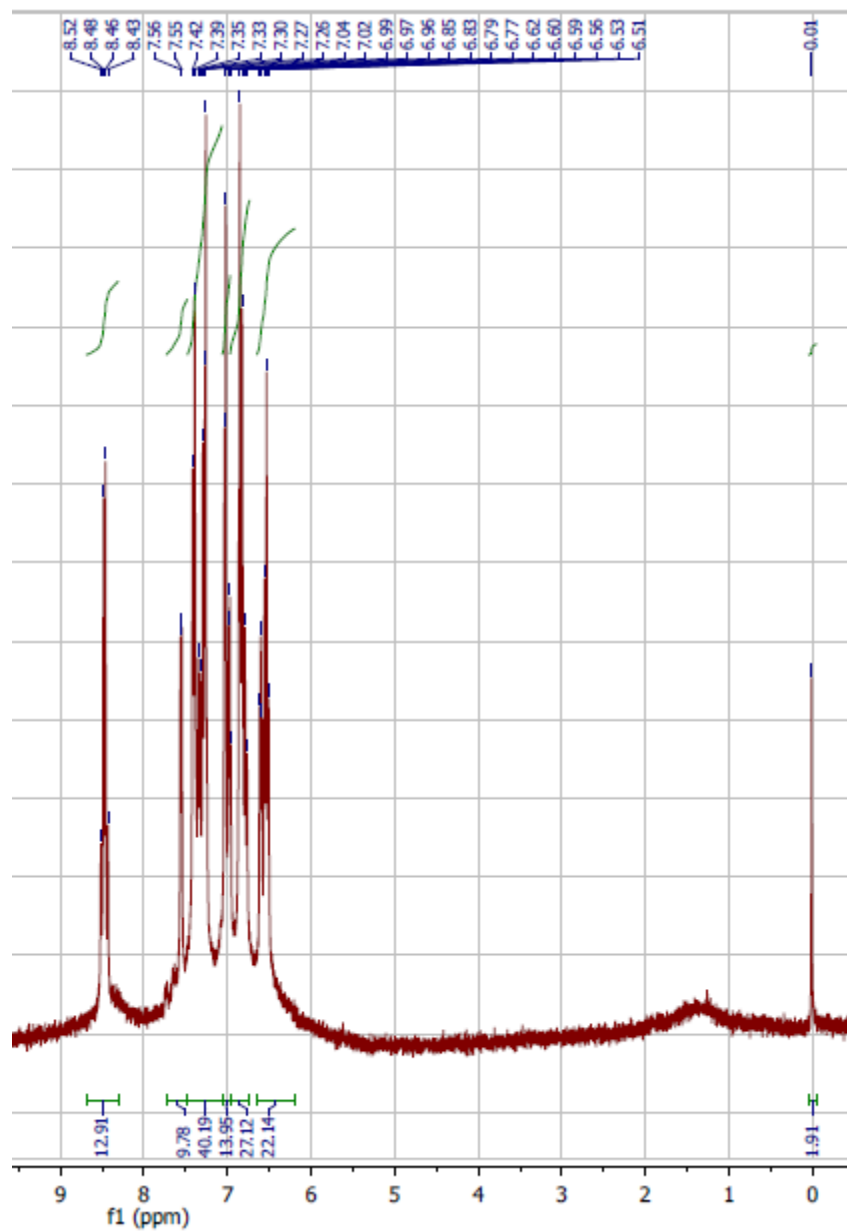


Fig. S5. $^1\text{H-NMR}$ spectrum of complex **2** in CDCl_3 .

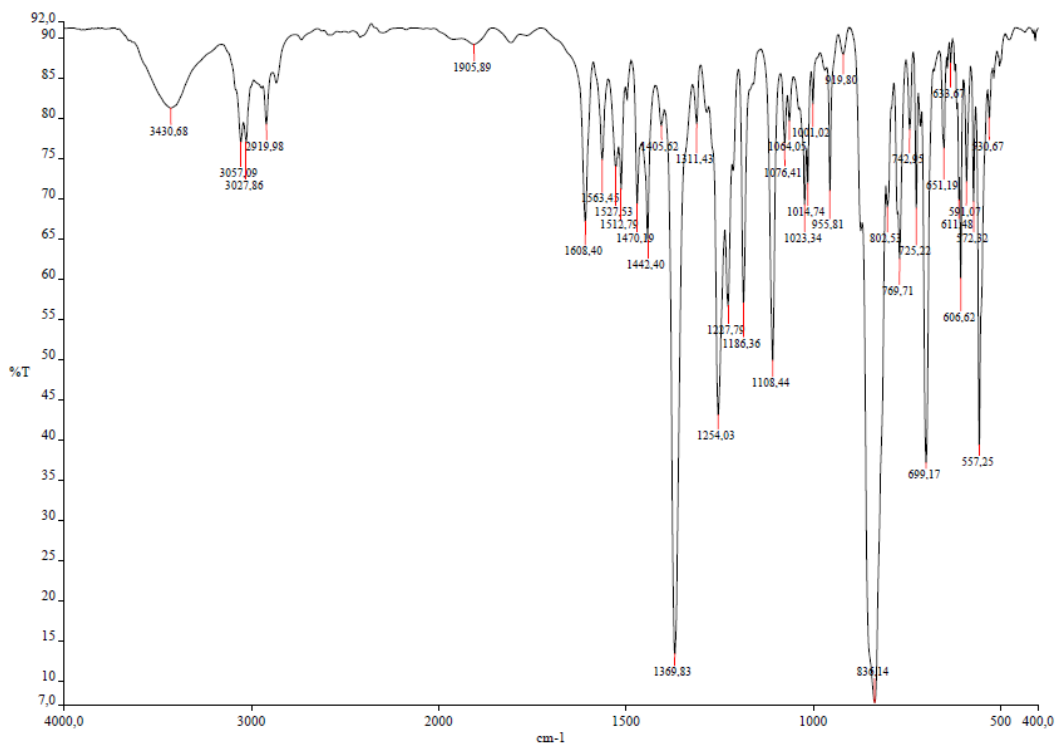


Fig. S6. The FT-IR spectrum of complex 1.

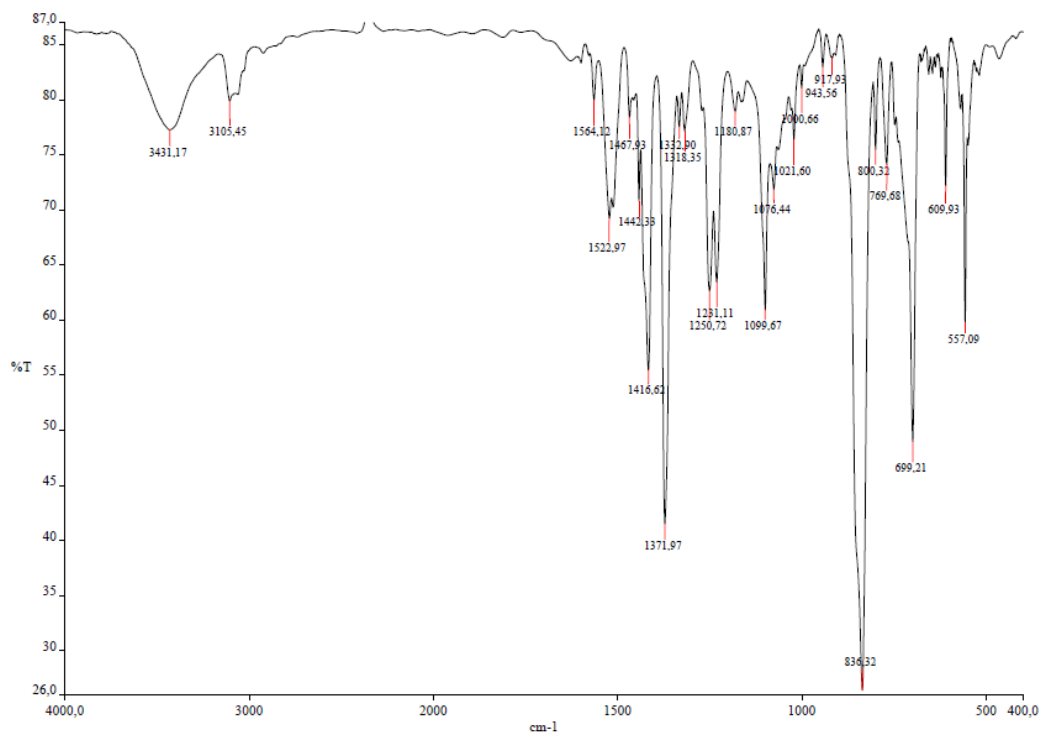


Fig. S7. The FT-IR spectrum of complex 2.

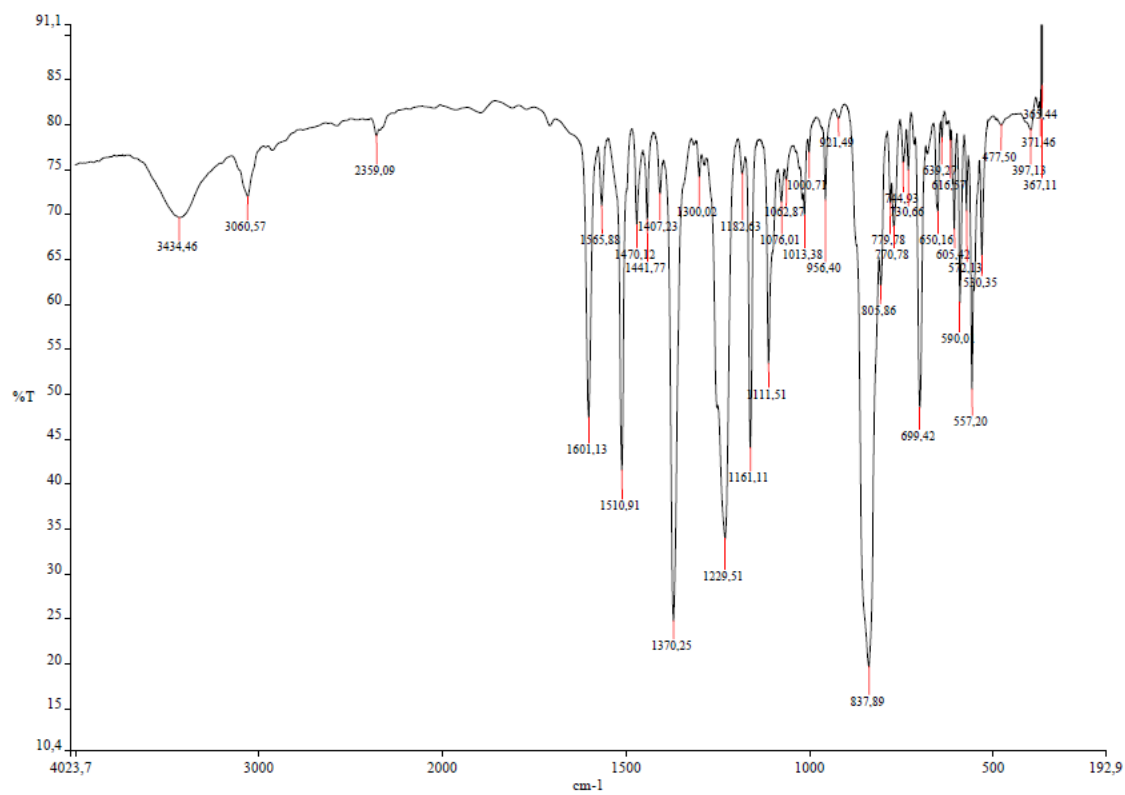


Fig. S8. The FT-IR spectrum of complex 3.

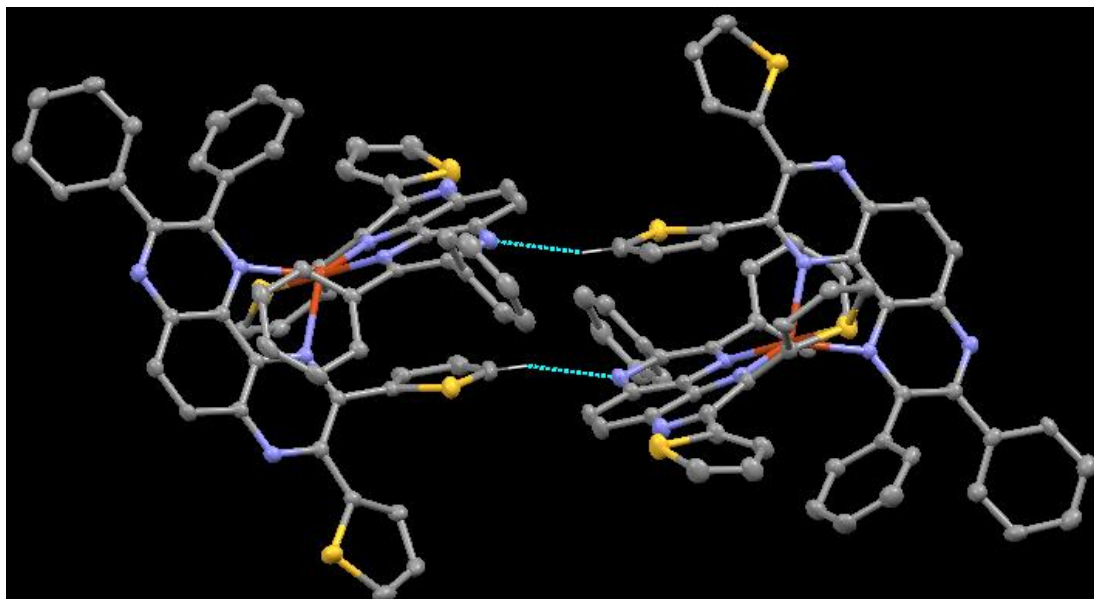


Fig. S9. The individual formation in complex 2 by pairs of intermolecular centrosymmetric C–H...N hydrogen bonds in complex 2.

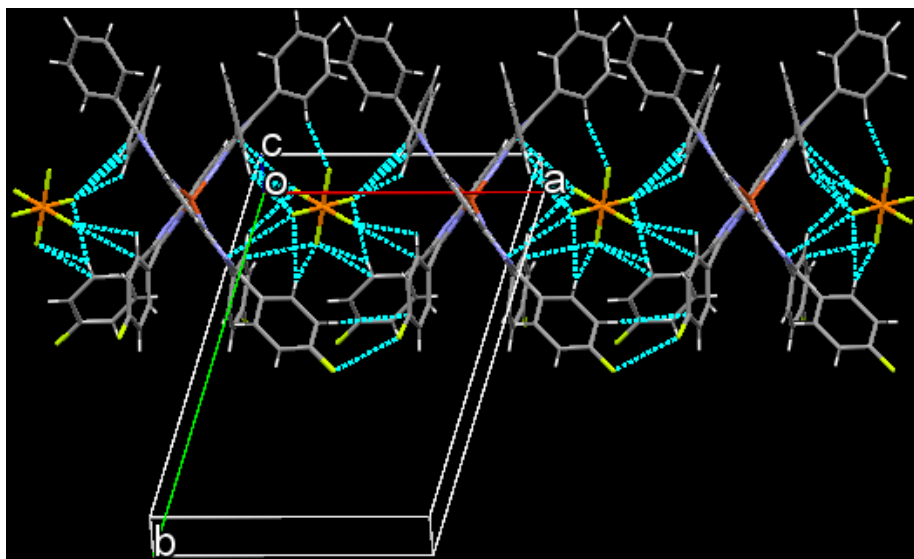


Fig. S10. Aggregation of cations and anions by the intermolecular C–H...F interactions which form a one-dimensional chain along the *a*-axis.

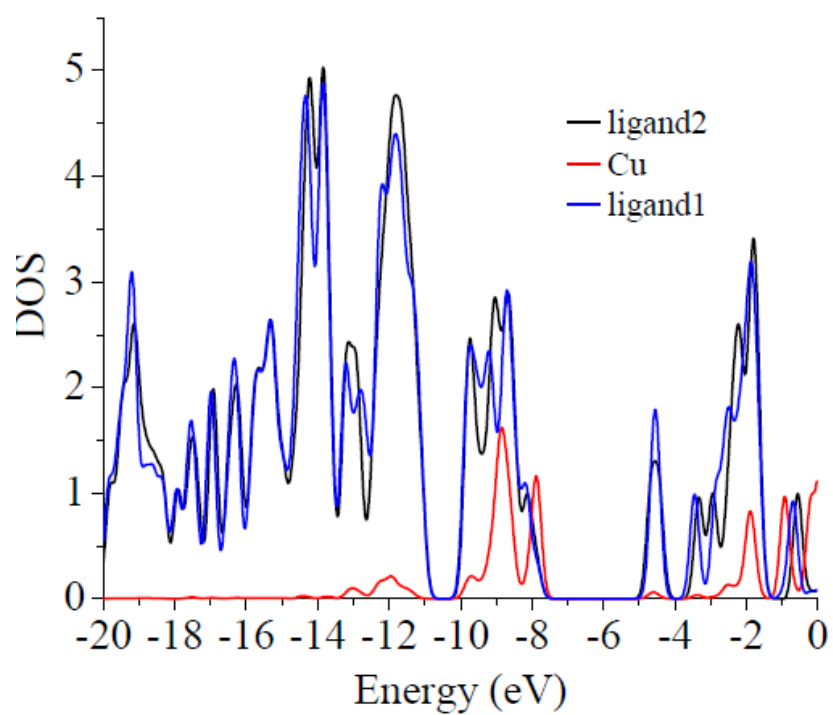


Fig. S11. Density of states (DOS) of complex **1** (each coordinated ligand considered differently as ligand 1 and ligand 2).

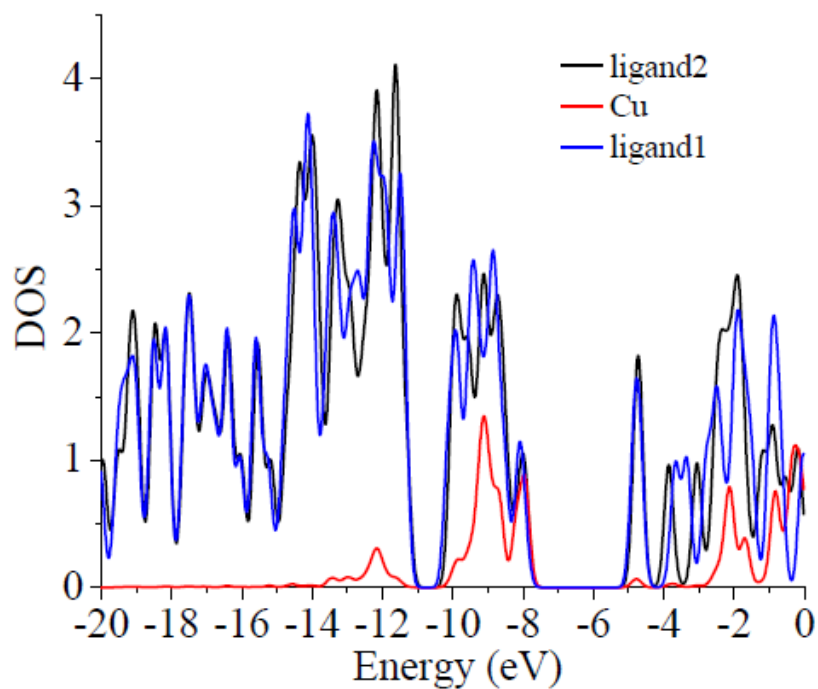


Fig. S12. Density of states (DOS) of complex 2 (each coordinated ligand considered differently as ligand 1 and ligand 2).

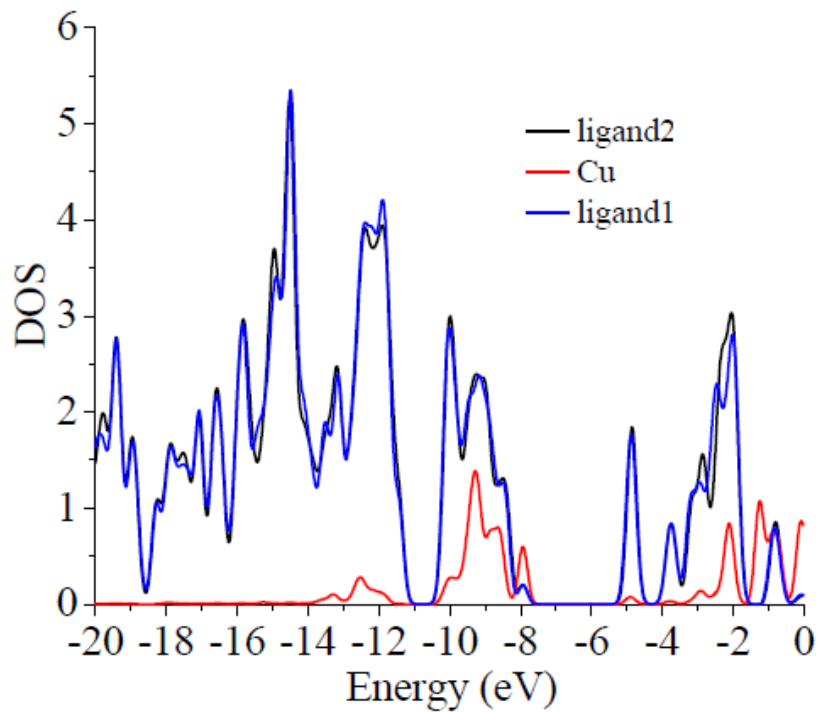


Fig. S13. Density of states (DOS) of complex 3 (each coordinated ligand considered differently as ligand 1 and ligand 2).

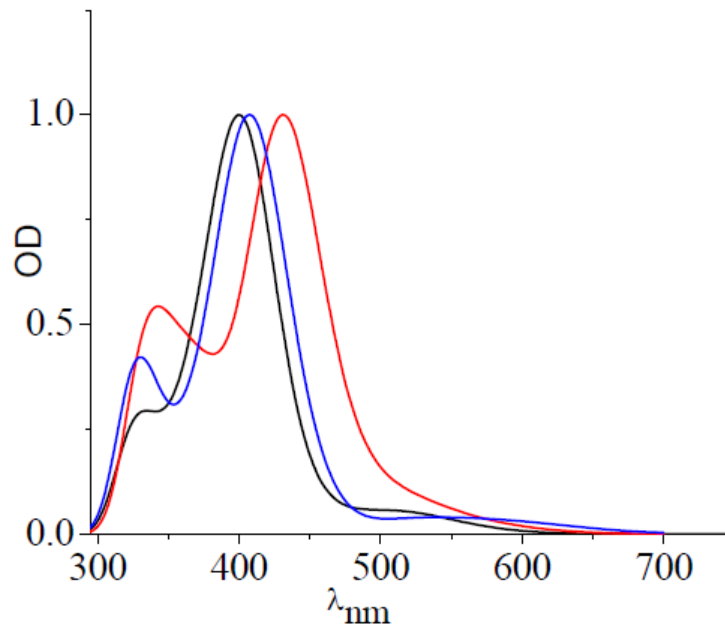


Fig. S14. Calculated UV-Vis spectra of complexes **1** (black), **2** (red) and **3** (blue).

Table 1. Crystal data and structure refinement for Complex 1.

Identification code	Complex 1	
Empirical formula	C ₇₂ H ₅₂ Cu F ₆ N ₈ P	
Formula weight	1237.73	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	<i>P</i> -1	
Unit cell dimensions	a = 12.7941(4) Å	α = 65.127(3)°
b = 16.0106(5) Å	β = 83.633(2)°.	
c = 16.0151(5) Å	γ = 85.192(3)°.	
Volume	2955.38(15) Å ³	
Z	2	
Density (calculated)	1.391 Mg/m ³	
Absorption coefficient	0.468 mm ⁻¹	
F(000)	1276	
Crystal size	0.25 x 0.15 x 0.10 mm ³	

Theta range for data collection	3.12 to 26.00°
Index ranges	-15<=h<=15, -17<=k<=19, -17<=l<=19
Reflections collected	22571
Independent reflections	11535 [R(int) = 0.0232]
Completeness to theta = 26.00°	99.3 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.8920
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11535 / 0 / 795
Goodness-of-fit on F ²	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1381
R indices (all data)	R1 = 0.0610, wR2 = 0.1437
Largest diff. peak and hole	2.034 and -1.072 e.Å ⁻³

Table 2. Bond lengths [\AA] and angles [$^\circ$] for sq.

C(1)-N(1)	1.332(3)
C(1)-C(2)	1.442(4)
C(1)-C(11)	1.482(4)
C(2)-N(5)	1.322(4)
C(2)-C(17)	1.490(4)
C(3)-N(5)	1.357(3)
C(3)-C(4)	1.405(4)
C(3)-C(8)	1.431(4)
C(4)-N(1)	1.361(3)
C(4)-C(5)	1.434(3)
C(5)-N(2)	1.354(3)
C(5)-C(6)	1.391(4)
C(6)-N(6)	1.356(3)
C(6)-C(7)	1.440(4)
C(7)-C(8)	1.356(4)
C(7)-H(7A)	0.9500
C(8)-H(8A)	0.9500
C(9)-N(6)	1.330(3)
C(9)-C(10)	1.439(4)
C(9)-C(30)	1.483(3)
C(10)-N(2)	1.328(3)
C(10)-C(23)	1.484(3)
C(11)-C(16)	1.396(4)
C(11)-C(12)	1.397(4)
C(12)-C(13)	1.384(4)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.388(5)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.383(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.392(4)
C(15)-H(15A)	0.9500
C(16)-H(16A)	0.9500
C(17)-C(22)	1.389(4)

C(17)-C(18)	1.393(4)
C(18)-C(19)	1.392(4)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.372(4)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.389(4)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.389(4)
C(21)-H(21A)	0.9500
C(22)-H(22A)	0.9500
C(23)-C(24)	1.393(4)
C(23)-C(28)	1.401(4)
C(24)-C(25)	1.387(4)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.391(4)
C(25)-H(25A)	0.9500
C(26)-C(27)	1.386(4)
C(26)-C(29)	1.506(4)
C(27)-C(28)	1.391(4)
C(27)-H(27A)	0.9500
C(28)-H(28A)	0.9500
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-C(31)	1.394(4)
C(30)-C(35)	1.396(4)
C(31)-C(32)	1.381(4)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.393(4)
C(32)-H(32A)	0.9500
C(33)-C(34)	1.393(4)
C(33)-C(36)	1.507(4)
C(34)-C(35)	1.388(4)
C(34)-H(34A)	0.9500
C(35)-H(35A)	0.9500
C(36)-H(36A)	0.9800

C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-N(3)	1.328(3)
C(37)-C(38)	1.438(4)
C(37)-C(47)	1.487(4)
C(38)-N(7)	1.333(4)
C(38)-C(53)	1.487(4)
C(39)-N(7)	1.349(4)
C(39)-C(40)	1.399(3)
C(39)-C(44)	1.434(4)
C(40)-N(3)	1.370(3)
C(40)-C(41)	1.429(4)
C(41)-N(4)	1.359(3)
C(41)-C(42)	1.406(4)
C(42)-N(8)	1.349(4)
C(42)-C(43)	1.436(4)
C(43)-C(44)	1.344(4)
C(43)-H(43A)	0.9500
C(44)-H(44A)	0.9500
C(45)-N(8)	1.332(3)
C(45)-C(46)	1.439(4)
C(45)-C(66)	1.481(4)
C(46)-N(4)	1.330(3)
C(46)-C(59)	1.493(3)
C(47)-C(52)	1.389(4)
C(47)-C(48)	1.389(4)
C(48)-C(49)	1.401(4)
C(48)-H(48A)	0.9500
C(49)-C(50)	1.379(6)
C(49)-H(49A)	0.9500
C(50)-C(51)	1.375(6)
C(50)-H(50A)	0.9500
C(51)-C(52)	1.399(4)
C(51)-H(51A)	0.9500
C(52)-H(52A)	0.9500
C(53)-C(54)	1.396(4)

C(53)-C(58)	1.398(4)
C(54)-C(55)	1.396(4)
C(54)-H(54A)	0.9500
C(55)-C(56)	1.383(5)
C(55)-H(55A)	0.9500
C(56)-C(57)	1.382(5)
C(56)-H(56A)	0.9500
C(57)-C(58)	1.386(4)
C(57)-H(57A)	0.9500
C(58)-H(58A)	0.9500
C(59)-C(64)	1.386(4)
C(59)-C(60)	1.402(4)
C(60)-C(61)	1.391(4)
C(60)-H(60A)	0.9500
C(61)-C(62)	1.393(4)
C(61)-H(61A)	0.9500
C(62)-C(63)	1.390(4)
C(62)-C(65)	1.502(4)
C(63)-C(64)	1.395(4)
C(63)-H(63A)	0.9500
C(64)-H(64A)	0.9500
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
C(66)-C(71)	1.389(4)
C(66)-C(67)	1.407(4)
C(67)-C(68)	1.381(4)
C(67)-H(67A)	0.9500
C(68)-C(69)	1.385(5)
C(68)-H(68A)	0.9500
C(69)-C(70)	1.400(4)
C(69)-C(72)	1.496(4)
C(70)-C(71)	1.385(4)
C(70)-H(70A)	0.9500
C(71)-H(71A)	0.9500
C(72)-H(72A)	0.9800

C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
N(1)-Cu(1)	2.027(2)
N(2)-Cu(1)	2.111(2)
N(3)-Cu(1)	2.002(2)
N(4)-Cu(1)	2.165(2)
F(1)-P(1)	1.607(2)
F(2)-P(1)	1.596(2)
F(3)-P(1)	1.583(3)
F(4)-P(1)	1.557(2)
F(6)-P(1)	1.597(2)
F(5)-P(1)	1.621(3)

N(1)-C(1)-C(2)	119.9(2)
N(1)-C(1)-C(11)	118.2(2)
C(2)-C(1)-C(11)	121.9(2)
N(5)-C(2)-C(1)	122.0(2)
N(5)-C(2)-C(17)	115.7(2)
C(1)-C(2)-C(17)	122.2(2)
N(5)-C(3)-C(4)	120.2(2)
N(5)-C(3)-C(8)	119.6(2)
C(4)-C(3)-C(8)	120.0(2)
N(1)-C(4)-C(3)	122.0(2)
N(1)-C(4)-C(5)	118.9(2)
C(3)-C(4)-C(5)	119.1(2)
N(2)-C(5)-C(6)	121.7(2)
N(2)-C(5)-C(4)	118.5(2)
C(6)-C(5)-C(4)	119.8(2)
N(6)-C(6)-C(5)	120.6(2)
N(6)-C(6)-C(7)	119.5(2)
C(5)-C(6)-C(7)	119.8(2)
C(8)-C(7)-C(6)	120.3(2)
C(8)-C(7)-H(7A)	119.8
C(6)-C(7)-H(7A)	119.8
C(7)-C(8)-C(3)	120.5(2)
C(7)-C(8)-H(8A)	119.7

C(3)-C(8)-H(8A)	119.7
N(6)-C(9)-C(10)	121.3(2)
N(6)-C(9)-C(30)	115.4(2)
C(10)-C(9)-C(30)	123.3(2)
N(2)-C(10)-C(9)	120.1(2)
N(2)-C(10)-C(23)	116.4(2)
C(9)-C(10)-C(23)	123.4(2)
C(16)-C(11)-C(12)	119.2(2)
C(16)-C(11)-C(1)	120.4(2)
C(12)-C(11)-C(1)	120.4(2)
C(13)-C(12)-C(11)	120.0(3)
C(13)-C(12)-H(12A)	120.0
C(11)-C(12)-H(12A)	120.0
C(12)-C(13)-C(14)	120.4(3)
C(12)-C(13)-H(13A)	119.8
C(14)-C(13)-H(13A)	119.8
C(15)-C(14)-C(13)	120.1(3)
C(15)-C(14)-H(14A)	120.0
C(13)-C(14)-H(14A)	120.0
C(14)-C(15)-C(16)	119.8(3)
C(14)-C(15)-H(15A)	120.1
C(16)-C(15)-H(15A)	120.1
C(15)-C(16)-C(11)	120.4(3)
C(15)-C(16)-H(16A)	119.8
C(11)-C(16)-H(16A)	119.8
C(22)-C(17)-C(18)	119.3(2)
C(22)-C(17)-C(2)	120.8(2)
C(18)-C(17)-C(2)	119.8(2)
C(19)-C(18)-C(17)	120.1(3)
C(19)-C(18)-H(18A)	119.9
C(17)-C(18)-H(18A)	119.9
C(20)-C(19)-C(18)	120.5(3)
C(20)-C(19)-H(19A)	119.8
C(18)-C(19)-H(19A)	119.8
C(19)-C(20)-C(21)	119.6(3)
C(19)-C(20)-H(20A)	120.2

C(21)-C(20)-H(20A)	120.2
C(20)-C(21)-C(22)	120.4(3)
C(20)-C(21)-H(21A)	119.8
C(22)-C(21)-H(21A)	119.8
C(17)-C(22)-C(21)	120.1(3)
C(17)-C(22)-H(22A)	120.0
C(21)-C(22)-H(22A)	120.0
C(24)-C(23)-C(28)	119.4(2)
C(24)-C(23)-C(10)	118.5(2)
C(28)-C(23)-C(10)	122.1(2)
C(25)-C(24)-C(23)	120.2(3)
C(25)-C(24)-H(24A)	119.9
C(23)-C(24)-H(24A)	119.9
C(24)-C(25)-C(26)	120.8(3)
C(24)-C(25)-H(25A)	119.6
C(26)-C(25)-H(25A)	119.6
C(27)-C(26)-C(25)	118.8(2)
C(27)-C(26)-C(29)	120.9(3)
C(25)-C(26)-C(29)	120.3(3)
C(26)-C(27)-C(28)	121.3(3)
C(26)-C(27)-H(27A)	119.4
C(28)-C(27)-H(27A)	119.4
C(27)-C(28)-C(23)	119.5(3)
C(27)-C(28)-H(28A)	120.2
C(23)-C(28)-H(28A)	120.2
C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-C(35)	119.1(2)
C(31)-C(30)-C(9)	117.5(2)
C(35)-C(30)-C(9)	123.2(2)
C(32)-C(31)-C(30)	120.4(3)
C(32)-C(31)-H(31A)	119.8

C(30)-C(31)-H(31A)	119.8
C(31)-C(32)-C(33)	120.9(3)
C(31)-C(32)-H(32A)	119.6
C(33)-C(32)-H(32A)	119.6
C(32)-C(33)-C(34)	118.6(3)
C(32)-C(33)-C(36)	120.7(3)
C(34)-C(33)-C(36)	120.7(3)
C(35)-C(34)-C(33)	120.9(3)
C(35)-C(34)-H(34A)	119.5
C(33)-C(34)-H(34A)	119.5
C(34)-C(35)-C(30)	120.0(3)
C(34)-C(35)-H(35A)	120.0
C(30)-C(35)-H(35A)	120.0
C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
N(3)-C(37)-C(38)	120.8(2)
N(3)-C(37)-C(47)	116.4(2)
C(38)-C(37)-C(47)	122.7(2)
N(7)-C(38)-C(37)	121.1(2)
N(7)-C(38)-C(53)	115.0(2)
C(37)-C(38)-C(53)	123.9(2)
N(7)-C(39)-C(40)	121.3(2)
N(7)-C(39)-C(44)	119.4(2)
C(40)-C(39)-C(44)	119.3(2)
N(3)-C(40)-C(39)	121.1(2)
N(3)-C(40)-C(41)	118.7(2)
C(39)-C(40)-C(41)	120.0(2)
N(4)-C(41)-C(42)	121.3(2)
N(4)-C(41)-C(40)	119.1(2)
C(42)-C(41)-C(40)	119.5(2)
N(8)-C(42)-C(41)	120.9(2)
N(8)-C(42)-C(43)	119.8(2)

C(41)-C(42)-C(43)	119.3(2)
C(44)-C(43)-C(42)	121.0(2)
C(44)-C(43)-H(43A)	119.5
C(42)-C(43)-H(43A)	119.5
C(43)-C(44)-C(39)	120.9(2)
C(43)-C(44)-H(44A)	119.5
C(39)-C(44)-H(44A)	119.5
N(8)-C(45)-C(46)	120.7(2)
N(8)-C(45)-C(66)	115.6(2)
C(46)-C(45)-C(66)	123.7(2)
N(4)-C(46)-C(45)	121.0(2)
N(4)-C(46)-C(59)	116.6(2)
C(45)-C(46)-C(59)	122.3(2)
C(52)-C(47)-C(48)	120.1(3)
C(52)-C(47)-C(37)	119.8(3)
C(48)-C(47)-C(37)	120.1(3)
C(47)-C(48)-C(49)	119.5(3)
C(47)-C(48)-H(48A)	120.3
C(49)-C(48)-H(48A)	120.3
C(50)-C(49)-C(48)	120.2(3)
C(50)-C(49)-H(49A)	119.9
C(48)-C(49)-H(49A)	119.9
C(51)-C(50)-C(49)	120.3(3)
C(51)-C(50)-H(50A)	119.8
C(49)-C(50)-H(50A)	119.8
C(50)-C(51)-C(52)	120.2(3)
C(50)-C(51)-H(51A)	119.9
C(52)-C(51)-H(51A)	119.9
C(47)-C(52)-C(51)	119.7(3)
C(47)-C(52)-H(52A)	120.2
C(51)-C(52)-H(52A)	120.2
C(54)-C(53)-C(58)	118.8(3)
C(54)-C(53)-C(38)	121.8(2)
C(58)-C(53)-C(38)	119.1(3)
C(55)-C(54)-C(53)	120.3(3)
C(55)-C(54)-H(54A)	119.8

C(53)-C(54)-H(54A)	119.8
C(56)-C(55)-C(54)	120.3(3)
C(56)-C(55)-H(55A)	119.8
C(54)-C(55)-H(55A)	119.8
C(57)-C(56)-C(55)	119.5(3)
C(57)-C(56)-H(56A)	120.2
C(55)-C(56)-H(56A)	120.2
C(56)-C(57)-C(58)	120.8(3)
C(56)-C(57)-H(57A)	119.6
C(58)-C(57)-H(57A)	119.6
C(57)-C(58)-C(53)	120.3(3)
C(57)-C(58)-H(58A)	119.8
C(53)-C(58)-H(58A)	119.8
C(64)-C(59)-C(60)	119.4(2)
C(64)-C(59)-C(46)	120.2(2)
C(60)-C(59)-C(46)	120.3(2)
C(61)-C(60)-C(59)	119.6(3)
C(61)-C(60)-H(60A)	120.2
C(59)-C(60)-H(60A)	120.2
C(60)-C(61)-C(62)	121.4(3)
C(60)-C(61)-H(61A)	119.3
C(62)-C(61)-H(61A)	119.3
C(63)-C(62)-C(61)	118.3(2)
C(63)-C(62)-C(65)	121.3(3)
C(61)-C(62)-C(65)	120.4(3)
C(62)-C(63)-C(64)	121.0(3)
C(62)-C(63)-H(63A)	119.5
C(64)-C(63)-H(63A)	119.5
C(59)-C(64)-C(63)	120.2(3)
C(59)-C(64)-H(64A)	119.9
C(63)-C(64)-H(64A)	119.9
C(62)-C(65)-H(65A)	109.5
C(62)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(62)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5

H(65B)-C(65)-H(65C)	109.5
C(71)-C(66)-C(67)	118.7(3)
C(71)-C(66)-C(45)	123.3(2)
C(67)-C(66)-C(45)	118.0(3)
C(68)-C(67)-C(66)	119.8(3)
C(68)-C(67)-H(67A)	120.1
C(66)-C(67)-H(67A)	120.1
C(67)-C(68)-C(69)	121.9(3)
C(67)-C(68)-H(68A)	119.0
C(69)-C(68)-H(68A)	119.0
C(68)-C(69)-C(70)	117.9(3)
C(68)-C(69)-C(72)	121.3(3)
C(70)-C(69)-C(72)	120.8(3)
C(71)-C(70)-C(69)	121.0(3)
C(71)-C(70)-H(70A)	119.5
C(69)-C(70)-H(70A)	119.5
C(70)-C(71)-C(66)	120.6(3)
C(70)-C(71)-H(71A)	119.7
C(66)-C(71)-H(71A)	119.7
C(69)-C(72)-H(72A)	109.5
C(69)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(69)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(1)-N(1)-C(4)	117.7(2)
C(1)-N(1)-Cu(1)	131.43(18)
C(4)-N(1)-Cu(1)	110.47(16)
C(10)-N(2)-C(5)	117.9(2)
C(10)-N(2)-Cu(1)	131.49(17)
C(5)-N(2)-Cu(1)	108.01(16)
C(37)-N(3)-C(40)	117.6(2)
C(37)-N(3)-Cu(1)	129.82(18)
C(40)-N(3)-Cu(1)	111.41(17)
C(46)-N(4)-C(41)	117.7(2)
C(46)-N(4)-Cu(1)	133.62(17)

C(41)-N(4)-Cu(1)	106.62(17)
C(2)-N(5)-C(3)	117.9(2)
C(9)-N(6)-C(6)	117.7(2)
C(38)-N(7)-C(39)	117.9(2)
C(45)-N(8)-C(42)	118.3(2)
F(4)-P(1)-F(3)	94.07(18)
F(4)-P(1)-F(2)	176.35(17)
F(3)-P(1)-F(2)	89.40(15)
F(4)-P(1)-F(6)	91.84(13)
F(3)-P(1)-F(6)	91.36(14)
F(2)-P(1)-F(6)	89.16(12)
F(4)-P(1)-F(1)	90.38(14)
F(3)-P(1)-F(1)	90.54(15)
F(2)-P(1)-F(1)	88.50(13)
F(6)-P(1)-F(1)	176.97(14)
F(4)-P(1)-F(5)	88.50(17)
F(3)-P(1)-F(5)	177.39(16)
F(2)-P(1)-F(5)	88.01(13)
F(6)-P(1)-F(5)	88.94(13)
F(1)-P(1)-F(5)	89.05(14)
N(3)-Cu(1)-N(1)	147.91(9)
N(3)-Cu(1)-N(2)	119.65(8)
N(1)-Cu(1)-N(2)	82.92(8)
N(3)-Cu(1)-N(4)	82.43(8)
N(1)-Cu(1)-N(4)	120.40(8)
N(2)-Cu(1)-N(4)	95.15(8)

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for sq.

N(1)-C(1)-C(2)-N(5)	-5.8(4)
C(11)-C(1)-C(2)-N(5)	173.9(3)
N(1)-C(1)-C(2)-C(17)	171.7(2)
C(11)-C(1)-C(2)-C(17)	-8.7(4)
N(5)-C(3)-C(4)-N(1)	-3.3(4)
C(8)-C(3)-C(4)-N(1)	-179.4(2)
N(5)-C(3)-C(4)-C(5)	175.5(2)
C(8)-C(3)-C(4)-C(5)	-0.6(4)
N(1)-C(4)-C(5)-N(2)	-5.4(4)
C(3)-C(4)-C(5)-N(2)	175.7(2)
N(1)-C(4)-C(5)-C(6)	173.4(2)
C(3)-C(4)-C(5)-C(6)	-5.4(4)
N(2)-C(5)-C(6)-N(6)	8.2(4)
C(4)-C(5)-C(6)-N(6)	-170.6(2)
N(2)-C(5)-C(6)-C(7)	-173.8(2)
C(4)-C(5)-C(6)-C(7)	7.4(4)
N(6)-C(6)-C(7)-C(8)	174.7(3)
C(5)-C(6)-C(7)-C(8)	-3.4(4)
C(6)-C(7)-C(8)-C(3)	-2.7(4)
N(5)-C(3)-C(8)-C(7)	-171.4(3)
C(4)-C(3)-C(8)-C(7)	4.7(4)
N(6)-C(9)-C(10)-N(2)	7.7(4)
C(30)-C(9)-C(10)-N(2)	-170.9(2)
N(6)-C(9)-C(10)-C(23)	-169.3(2)
C(30)-C(9)-C(10)-C(23)	12.1(4)
N(1)-C(1)-C(11)-C(16)	-47.4(4)
C(2)-C(1)-C(11)-C(16)	132.9(3)
N(1)-C(1)-C(11)-C(12)	131.9(3)
C(2)-C(1)-C(11)-C(12)	-47.7(4)
C(16)-C(11)-C(12)-C(13)	-0.8(4)
C(1)-C(11)-C(12)-C(13)	179.8(3)
C(11)-C(12)-C(13)-C(14)	-1.1(5)
C(12)-C(13)-C(14)-C(15)	1.9(5)
C(13)-C(14)-C(15)-C(16)	-0.8(5)

C(14)-C(15)-C(16)-C(11)	-1.2(4)
C(12)-C(11)-C(16)-C(15)	2.0(4)
C(1)-C(11)-C(16)-C(15)	-178.7(3)
N(5)-C(2)-C(17)-C(22)	130.2(3)
C(1)-C(2)-C(17)-C(22)	-47.4(4)
N(5)-C(2)-C(17)-C(18)	-46.2(4)
C(1)-C(2)-C(17)-C(18)	136.2(3)
C(22)-C(17)-C(18)-C(19)	2.4(5)
C(2)-C(17)-C(18)-C(19)	178.7(3)
C(17)-C(18)-C(19)-C(20)	-1.7(5)
C(18)-C(19)-C(20)-C(21)	-0.5(5)
C(19)-C(20)-C(21)-C(22)	2.1(5)
C(18)-C(17)-C(22)-C(21)	-0.8(4)
C(2)-C(17)-C(22)-C(21)	-177.1(3)
C(20)-C(21)-C(22)-C(17)	-1.4(5)
N(2)-C(10)-C(23)-C(24)	-57.6(3)
C(9)-C(10)-C(23)-C(24)	119.5(3)
N(2)-C(10)-C(23)-C(28)	122.2(3)
C(9)-C(10)-C(23)-C(28)	-60.7(4)
C(28)-C(23)-C(24)-C(25)	0.9(4)
C(10)-C(23)-C(24)-C(25)	-179.3(2)
C(23)-C(24)-C(25)-C(26)	-1.5(4)
C(24)-C(25)-C(26)-C(27)	0.9(4)
C(24)-C(25)-C(26)-C(29)	-178.7(3)
C(25)-C(26)-C(27)-C(28)	0.2(4)
C(29)-C(26)-C(27)-C(28)	179.8(2)
C(26)-C(27)-C(28)-C(23)	-0.7(4)
C(24)-C(23)-C(28)-C(27)	0.2(4)
C(10)-C(23)-C(28)-C(27)	-179.6(2)
N(6)-C(9)-C(30)-C(31)	-48.6(3)
C(10)-C(9)-C(30)-C(31)	130.1(3)
N(6)-C(9)-C(30)-C(35)	126.9(3)
C(10)-C(9)-C(30)-C(35)	-54.4(4)
C(35)-C(30)-C(31)-C(32)	1.0(4)
C(9)-C(30)-C(31)-C(32)	176.7(2)
C(30)-C(31)-C(32)-C(33)	-2.5(4)

C(31)-C(32)-C(33)-C(34)	1.4(4)
C(31)-C(32)-C(33)-C(36)	-179.8(3)
C(32)-C(33)-C(34)-C(35)	1.3(4)
C(36)-C(33)-C(34)-C(35)	-177.6(3)
C(33)-C(34)-C(35)-C(30)	-2.7(4)
C(31)-C(30)-C(35)-C(34)	1.6(4)
C(9)-C(30)-C(35)-C(34)	-173.8(2)
N(3)-C(37)-C(38)-N(7)	3.6(4)
C(47)-C(37)-C(38)-N(7)	-173.5(2)
N(3)-C(37)-C(38)-C(53)	-175.9(2)
C(47)-C(37)-C(38)-C(53)	7.0(4)
N(7)-C(39)-C(40)-N(3)	3.7(4)
C(44)-C(39)-C(40)-N(3)	-176.5(2)
N(7)-C(39)-C(40)-C(41)	179.1(2)
C(44)-C(39)-C(40)-C(41)	-1.0(4)
N(3)-C(40)-C(41)-N(4)	0.2(3)
C(39)-C(40)-C(41)-N(4)	-175.4(2)
N(3)-C(40)-C(41)-C(42)	175.4(2)
C(39)-C(40)-C(41)-C(42)	-0.2(4)
N(4)-C(41)-C(42)-N(8)	-2.7(4)
C(40)-C(41)-C(42)-N(8)	-177.8(2)
N(4)-C(41)-C(42)-C(43)	176.3(2)
C(40)-C(41)-C(42)-C(43)	1.2(4)
N(8)-C(42)-C(43)-C(44)	178.0(2)
C(41)-C(42)-C(43)-C(44)	-1.1(4)
C(42)-C(43)-C(44)-C(39)	-0.1(4)
N(7)-C(39)-C(44)-C(43)	-179.0(2)
C(40)-C(39)-C(44)-C(43)	1.2(4)
N(8)-C(45)-C(46)-N(4)	-2.0(4)
C(66)-C(45)-C(46)-N(4)	178.9(2)
N(8)-C(45)-C(46)-C(59)	174.6(2)
C(66)-C(45)-C(46)-C(59)	-4.5(4)
N(3)-C(37)-C(47)-C(52)	-111.3(3)
C(38)-C(37)-C(47)-C(52)	66.0(3)
N(3)-C(37)-C(47)-C(48)	67.7(3)
C(38)-C(37)-C(47)-C(48)	-115.1(3)

C(52)-C(47)-C(48)-C(49)	-1.8(4)
C(37)-C(47)-C(48)-C(49)	179.2(3)
C(47)-C(48)-C(49)-C(50)	1.8(5)
C(48)-C(49)-C(50)-C(51)	0.2(5)
C(49)-C(50)-C(51)-C(52)	-2.2(5)
C(48)-C(47)-C(52)-C(51)	-0.2(4)
C(37)-C(47)-C(52)-C(51)	178.8(3)
C(50)-C(51)-C(52)-C(47)	2.2(4)
N(7)-C(38)-C(53)-C(54)	-138.7(3)
C(37)-C(38)-C(53)-C(54)	40.8(4)
N(7)-C(38)-C(53)-C(58)	34.7(4)
C(37)-C(38)-C(53)-C(58)	-145.8(3)
C(58)-C(53)-C(54)-C(55)	0.2(4)
C(38)-C(53)-C(54)-C(55)	173.6(3)
C(53)-C(54)-C(55)-C(56)	-0.1(4)
C(54)-C(55)-C(56)-C(57)	0.1(5)
C(55)-C(56)-C(57)-C(58)	-0.2(5)
C(56)-C(57)-C(58)-C(53)	0.3(5)
C(54)-C(53)-C(58)-C(57)	-0.3(4)
C(38)-C(53)-C(58)-C(57)	-173.9(3)
N(4)-C(46)-C(59)-C(64)	115.6(3)
C(45)-C(46)-C(59)-C(64)	-61.2(4)
N(4)-C(46)-C(59)-C(60)	-61.9(3)
C(45)-C(46)-C(59)-C(60)	121.3(3)
C(64)-C(59)-C(60)-C(61)	1.3(4)
C(46)-C(59)-C(60)-C(61)	178.9(2)
C(59)-C(60)-C(61)-C(62)	-1.6(4)
C(60)-C(61)-C(62)-C(63)	0.3(4)
C(60)-C(61)-C(62)-C(65)	179.8(3)
C(61)-C(62)-C(63)-C(64)	1.2(4)
C(65)-C(62)-C(63)-C(64)	-178.3(3)
C(60)-C(59)-C(64)-C(63)	0.2(4)
C(46)-C(59)-C(64)-C(63)	-177.4(3)
C(62)-C(63)-C(64)-C(59)	-1.5(4)
N(8)-C(45)-C(66)-C(71)	135.4(3)
C(46)-C(45)-C(66)-C(71)	-45.5(4)

N(8)-C(45)-C(66)-C(67)	-42.1(4)
C(46)-C(45)-C(66)-C(67)	137.0(3)
C(71)-C(66)-C(67)-C(68)	1.1(4)
C(45)-C(66)-C(67)-C(68)	178.7(3)
C(66)-C(67)-C(68)-C(69)	-1.5(5)
C(67)-C(68)-C(69)-C(70)	-0.1(5)
C(67)-C(68)-C(69)-C(72)	177.5(3)
C(68)-C(69)-C(70)-C(71)	2.2(4)
C(72)-C(69)-C(70)-C(71)	-175.4(3)
C(69)-C(70)-C(71)-C(66)	-2.7(4)
C(67)-C(66)-C(71)-C(70)	1.0(4)
C(45)-C(66)-C(71)-C(70)	-176.5(2)
C(2)-C(1)-N(1)-C(4)	2.2(4)
C(11)-C(1)-N(1)-C(4)	-177.4(2)
C(2)-C(1)-N(1)-Cu(1)	-169.17(19)
C(11)-C(1)-N(1)-Cu(1)	11.2(4)
C(3)-C(4)-N(1)-C(1)	2.1(4)
C(5)-C(4)-N(1)-C(1)	-176.7(2)
C(3)-C(4)-N(1)-Cu(1)	175.2(2)
C(5)-C(4)-N(1)-Cu(1)	-3.6(3)
C(9)-C(10)-N(2)-C(5)	-3.4(4)
C(23)-C(10)-N(2)-C(5)	173.8(2)
C(9)-C(10)-N(2)-Cu(1)	155.86(19)
C(23)-C(10)-N(2)-Cu(1)	-27.0(3)
C(6)-C(5)-N(2)-C(10)	-4.2(4)
C(4)-C(5)-N(2)-C(10)	174.6(2)
C(6)-C(5)-N(2)-Cu(1)	-168.0(2)
C(4)-C(5)-N(2)-Cu(1)	10.8(3)
C(38)-C(37)-N(3)-C(40)	0.1(4)
C(47)-C(37)-N(3)-C(40)	177.4(2)
C(38)-C(37)-N(3)-Cu(1)	-166.43(18)
C(47)-C(37)-N(3)-Cu(1)	10.9(3)
C(39)-C(40)-N(3)-C(37)	-3.5(4)
C(41)-C(40)-N(3)-C(37)	-179.1(2)
C(39)-C(40)-N(3)-Cu(1)	165.35(19)
C(41)-C(40)-N(3)-Cu(1)	-10.2(3)

C(45)-C(46)-N(4)-C(41)	2.7(3)
C(59)-C(46)-N(4)-C(41)	-174.1(2)
C(45)-C(46)-N(4)-Cu(1)	163.75(18)
C(59)-C(46)-N(4)-Cu(1)	-13.1(3)
C(42)-C(41)-N(4)-C(46)	-0.5(3)
C(40)-C(41)-N(4)-C(46)	174.6(2)
C(42)-C(41)-N(4)-Cu(1)	-166.2(2)
C(40)-C(41)-N(4)-Cu(1)	8.9(3)
C(1)-C(2)-N(5)-C(3)	4.5(4)
C(17)-C(2)-N(5)-C(3)	-173.1(2)
C(4)-C(3)-N(5)-C(2)	-0.1(4)
C(8)-C(3)-N(5)-C(2)	176.0(3)
C(10)-C(9)-N(6)-C(6)	-3.7(4)
C(30)-C(9)-N(6)-C(6)	175.0(2)
C(5)-C(6)-N(6)-C(9)	-3.9(4)
C(7)-C(6)-N(6)-C(9)	178.1(2)
C(37)-C(38)-N(7)-C(39)	-3.5(4)
C(53)-C(38)-N(7)-C(39)	176.0(2)
C(40)-C(39)-N(7)-C(38)	0.0(4)
C(44)-C(39)-N(7)-C(38)	-179.9(2)
C(46)-C(45)-N(8)-C(42)	-1.2(4)
C(66)-C(45)-N(8)-C(42)	178.0(2)
C(41)-C(42)-N(8)-C(45)	3.4(4)
C(43)-C(42)-N(8)-C(45)	-175.6(2)
C(37)-N(3)-Cu(1)-N(1)	-43.0(3)
C(40)-N(3)-Cu(1)-N(1)	149.81(17)
C(37)-N(3)-Cu(1)-N(2)	86.8(2)
C(40)-N(3)-Cu(1)-N(2)	-80.34(18)
C(37)-N(3)-Cu(1)-N(4)	178.5(2)
C(40)-N(3)-Cu(1)-N(4)	11.30(17)
C(1)-N(1)-Cu(1)-N(3)	-43.2(3)
C(4)-N(1)-Cu(1)-N(3)	144.96(18)
C(1)-N(1)-Cu(1)-N(2)	179.1(2)
C(4)-N(1)-Cu(1)-N(2)	7.20(17)
C(1)-N(1)-Cu(1)-N(4)	87.3(2)
C(4)-N(1)-Cu(1)-N(4)	-84.63(18)

C(10)-N(2)-Cu(1)-N(3)	33.7(3)
C(5)-N(2)-Cu(1)-N(3)	-165.48(16)
C(10)-N(2)-Cu(1)-N(1)	-170.5(2)
C(5)-N(2)-Cu(1)-N(1)	-9.74(17)
C(10)-N(2)-Cu(1)-N(4)	-50.5(2)
C(5)-N(2)-Cu(1)-N(4)	110.31(17)
C(46)-N(4)-Cu(1)-N(3)	-173.4(2)
C(41)-N(4)-Cu(1)-N(3)	-10.91(16)
C(46)-N(4)-Cu(1)-N(1)	30.7(3)
C(41)-N(4)-Cu(1)-N(1)	-166.83(15)
C(46)-N(4)-Cu(1)-N(2)	-54.1(2)
C(41)-N(4)-Cu(1)-N(2)	108.37(16)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for **Complex 2**.

Identification code	Complex 2	
Empirical formula	C ₆₀ H ₃₆ Cu F ₆ N ₈ P S ₄	
Formula weight	1205.72	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.4680(4) Å	α = 105.236(3)°.
	b = 13.3364(4) Å	β = 99.745(3)°.
	c = 17.4525(5) Å	γ = 106.481(3)°.
Volume	2590.02(14) Å ³	
Z	2	
Density (calculated)	1.546 Mg/m ³	
Absorption coefficient	3.013 mm ⁻¹	
F(000)	1228	
Crystal size	0.15 x 0.08 x 0.04 mm ³	
Theta range for data collection	3.66 to 72.50°	
Index ranges	-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -20 ≤ l ≤ 21	
Reflections collected	29380	
Independent reflections	10140 [R(int) = 0.0330]	

Completeness to theta = 72.50°	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.0000 and 0.6607
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	10140 / 0 / 724
Goodness-of-fit on F ²	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0399, wR2 = 0.1090
R indices (all data)	R1 = 0.0459, wR2 = 0.1139
Largest diff. peak and hole	0.678 and -0.599 e.Å ⁻³

Table 2. Bond lengths [\AA] and angles [$^\circ$] for a.

C(1)-N(1)	1.335(3)
C(1)-C(2)	1.439(3)
C(1)-C(11)	1.484(3)
C(2)-N(5)	1.334(3)
C(2)-C(17)	1.488(3)
C(3)-N(5)	1.350(3)
C(3)-C(4)	1.398(3)
C(3)-C(8)	1.440(3)
C(4)-N(1)	1.354(3)
C(4)-C(5)	1.430(3)
C(5)-N(2)	1.354(3)
C(5)-C(6)	1.400(3)
C(6)-N(6)	1.352(3)
C(6)-C(7)	1.436(3)
C(7)-C(8)	1.357(3)
C(7)-H(7A)	0.9500
C(8)-H(8A)	0.9500
C(9)-N(6)	1.340(3)
C(9)-C(10)	1.436(3)
C(9)-C(27)	1.462(3)
C(10)-N(2)	1.325(3)
C(10)-C(23)	1.471(3)
C(11)-C(12)	1.395(3)
C(11)-C(16)	1.429(3)
C(12)-C(13)	1.386(3)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.383(4)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.374(4)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.340(4)
C(15)-H(15A)	0.9500
C(16)-H(16A)	0.9500
C(17)-C(18)	1.393(3)

C(17)-C(22)	1.437(3)
C(18)-C(19)	1.388(3)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.389(4)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.371(4)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.329(3)
C(21)-H(21A)	0.9500
C(22)-H(22A)	0.9500
C(23)-C(24)	1.383(3)
C(23)-S(1)	1.733(2)
C(24)-C(25)	1.448(3)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.362(4)
C(25)-H(25A)	0.9500
C(26)-S(1)	1.701(3)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.387(3)
C(27)-S(2)	1.729(2)
C(28)-C(29)	1.413(3)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.356(4)
C(29)-H(29A)	0.9500
C(30)-S(2)	1.721(3)
C(30)-H(30A)	0.9500
C(31)-N(3)	1.332(3)
C(31)-C(32)	1.431(3)
C(31)-C(41)	1.488(3)
C(32)-N(7)	1.330(3)
C(32)-C(47)	1.489(3)
C(33)-N(7)	1.354(3)
C(33)-C(34)	1.402(3)
C(33)-C(38)	1.429(3)
C(34)-N(3)	1.361(3)
C(34)-C(35)	1.431(3)

C(35)-N(4)	1.366(3)
C(35)-C(36)	1.399(3)
C(36)-N(8)	1.350(3)
C(36)-C(37)	1.429(3)
C(37)-C(38)	1.354(3)
C(37)-H(37A)	0.9500
C(38)-H(38A)	0.9500
C(39)-N(8)	1.326(3)
C(39)-C(40)	1.447(3)
C(39)-C(57)	1.464(3)
C(40)-N(4)	1.342(3)
C(40)-C(53)	1.460(3)
C(41)-C(42)	1.389(3)
C(41)-C(46)	1.409(3)
C(42)-C(43)	1.395(3)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.382(4)
C(43)-H(43A)	0.9500
C(44)-C(45)	1.383(4)
C(44)-H(44A)	0.9500
C(45)-C(46)	1.384(3)
C(45)-H(45A)	0.9500
C(46)-H(46A)	0.9500
C(47)-C(52)	1.393(3)
C(47)-C(48)	1.394(3)
C(48)-C(49)	1.394(3)
C(48)-H(48A)	0.9500
C(49)-C(50)	1.383(4)
C(49)-H(49A)	0.9500
C(50)-C(51)	1.391(4)
C(50)-H(50A)	0.9500
C(51)-C(52)	1.382(3)
C(51)-H(51A)	0.9500
C(52)-H(52A)	0.9500
C(53)-C(54)	1.433(3)
C(53)-S(3)	1.732(2)

C(54)-C(55)	1.445(3)
C(54)-H(54A)	0.9500
C(55)-C(56)	1.356(3)
C(55)-H(55A)	0.9500
C(56)-S(3)	1.691(3)
C(56)-H(56A)	0.9500
C(57)-C(58)	1.377(3)
C(57)-S(4)	1.728(2)
C(58)-C(59)	1.420(3)
C(58)-H(58A)	0.9500
C(59)-C(60)	1.367(4)
C(59)-H(59A)	0.9500
C(60)-S(4)	1.704(3)
C(60)-H(60A)	0.9500
N(1)-Cu(1)	2.0476(17)
N(2)-Cu(1)	2.0510(17)
N(3)-Cu(1)	2.0875(18)
N(4)-Cu(1)	2.0149(17)
F(1)-P(1)	1.6104(14)
F(2)-P(1)	1.5984(14)
F(3)-P(1)	1.6041(13)
F(4)-P(2)	1.6073(13)
F(5)-P(2)	1.6011(13)
F(6)-P(2)	1.6082(13)
P(1)-F(2)#1	1.5984(14)
P(1)-F(3)#1	1.6041(14)
P(1)-F(1)#1	1.6103(14)
P(2)-F(5)#2	1.6011(13)
P(2)-F(4)#2	1.6073(13)
P(2)-F(6)#2	1.6081(14)
N(1)-C(1)-C(2)	120.07(19)
N(1)-C(1)-C(11)	114.50(17)
C(2)-C(1)-C(11)	125.36(19)
N(5)-C(2)-C(1)	121.01(19)
N(5)-C(2)-C(17)	115.58(18)

C(1)-C(2)-C(17)	123.40(19)
N(5)-C(3)-C(4)	120.42(19)
N(5)-C(3)-C(8)	120.76(18)
C(4)-C(3)-C(8)	118.78(19)
N(1)-C(4)-C(3)	121.83(19)
N(1)-C(4)-C(5)	118.47(18)
C(3)-C(4)-C(5)	119.70(19)
N(2)-C(5)-C(6)	121.68(19)
N(2)-C(5)-C(4)	117.57(18)
C(6)-C(5)-C(4)	120.71(18)
N(6)-C(6)-C(5)	120.41(19)
N(6)-C(6)-C(7)	120.78(19)
C(5)-C(6)-C(7)	118.81(19)
C(8)-C(7)-C(6)	120.52(19)
C(8)-C(7)-H(7A)	119.7
C(6)-C(7)-H(7A)	119.7
C(7)-C(8)-C(3)	121.46(19)
C(7)-C(8)-H(8A)	119.3
C(3)-C(8)-H(8A)	119.3
N(6)-C(9)-C(10)	121.32(19)
N(6)-C(9)-C(27)	115.35(19)
C(10)-C(9)-C(27)	123.33(19)
N(2)-C(10)-C(9)	119.98(18)
N(2)-C(10)-C(23)	115.29(18)
C(9)-C(10)-C(23)	124.74(19)
C(12)-C(11)-C(16)	118.2(2)
C(12)-C(11)-C(1)	120.74(19)
C(16)-C(11)-C(1)	120.9(2)
C(13)-C(12)-C(11)	120.0(2)
C(13)-C(12)-H(12A)	120.0
C(11)-C(12)-H(12A)	120.0
C(14)-C(13)-C(12)	119.7(2)
C(14)-C(13)-H(13A)	120.2
C(12)-C(13)-H(13A)	120.2
C(15)-C(14)-C(13)	120.9(2)
C(15)-C(14)-H(14A)	119.6

C(13)-C(14)-H(14A)	119.6
C(16)-C(15)-C(14)	120.5(2)
C(16)-C(15)-H(15A)	119.8
C(14)-C(15)-H(15A)	119.8
C(15)-C(16)-C(11)	120.7(2)
C(15)-C(16)-H(16A)	119.6
C(11)-C(16)-H(16A)	119.6
C(18)-C(17)-C(22)	116.5(2)
C(18)-C(17)-C(2)	124.3(2)
C(22)-C(17)-C(2)	119.2(2)
C(19)-C(18)-C(17)	120.4(2)
C(19)-C(18)-H(18A)	119.8
C(17)-C(18)-H(18A)	119.8
C(18)-C(19)-C(20)	120.0(2)
C(18)-C(19)-H(19A)	120.0
C(20)-C(19)-H(19A)	120.0
C(21)-C(20)-C(19)	120.6(2)
C(21)-C(20)-H(20A)	119.7
C(19)-C(20)-H(20A)	119.7
C(22)-C(21)-C(20)	119.8(2)
C(22)-C(21)-H(21A)	120.1
C(20)-C(21)-H(21A)	120.1
C(21)-C(22)-C(17)	122.7(2)
C(21)-C(22)-H(22A)	118.6
C(17)-C(22)-H(22A)	118.6
C(24)-C(23)-C(10)	126.8(2)
C(24)-C(23)-S(1)	111.69(16)
C(10)-C(23)-S(1)	121.32(16)
C(23)-C(24)-C(25)	110.7(2)
C(23)-C(24)-H(24A)	124.6
C(25)-C(24)-H(24A)	124.6
C(26)-C(25)-C(24)	113.2(2)
C(26)-C(25)-H(25A)	123.4
C(24)-C(25)-H(25A)	123.4
C(25)-C(26)-S(1)	112.24(18)
C(25)-C(26)-H(26A)	123.9

S(1)-C(26)-H(26A)	123.9
C(28)-C(27)-C(9)	131.7(2)
C(28)-C(27)-S(2)	110.22(17)
C(9)-C(27)-S(2)	117.96(16)
C(27)-C(28)-C(29)	112.8(2)
C(27)-C(28)-H(28A)	123.6
C(29)-C(28)-H(28A)	123.6
C(30)-C(29)-C(28)	113.2(2)
C(30)-C(29)-H(29A)	123.4
C(28)-C(29)-H(29A)	123.4
C(29)-C(30)-S(2)	111.55(18)
C(29)-C(30)-H(30A)	124.2
S(2)-C(30)-H(30A)	124.2
N(3)-C(31)-C(32)	120.32(18)
N(3)-C(31)-C(41)	117.52(18)
C(32)-C(31)-C(41)	122.12(18)
N(7)-C(32)-C(31)	121.89(19)
N(7)-C(32)-C(47)	113.67(19)
C(31)-C(32)-C(47)	124.43(18)
N(7)-C(33)-C(34)	120.43(19)
N(7)-C(33)-C(38)	119.1(2)
C(34)-C(33)-C(38)	120.4(2)
N(3)-C(34)-C(33)	121.81(19)
N(3)-C(34)-C(35)	118.81(19)
C(33)-C(34)-C(35)	119.21(18)
N(4)-C(35)-C(36)	121.29(19)
N(4)-C(35)-C(34)	119.10(18)
C(36)-C(35)-C(34)	119.18(19)
N(8)-C(36)-C(35)	120.7(2)
N(8)-C(36)-C(37)	119.07(19)
C(35)-C(36)-C(37)	120.2(2)
C(38)-C(37)-C(36)	120.8(2)
C(38)-C(37)-H(37A)	119.6
C(36)-C(37)-H(37A)	119.6
C(37)-C(38)-C(33)	119.9(2)
C(37)-C(38)-H(38A)	120.0

C(33)-C(38)-H(38A)	120.0
N(8)-C(39)-C(40)	121.25(19)
N(8)-C(39)-C(57)	114.78(19)
C(40)-C(39)-C(57)	124.0(2)
N(4)-C(40)-C(39)	119.35(19)
N(4)-C(40)-C(53)	118.15(18)
C(39)-C(40)-C(53)	122.17(19)
C(42)-C(41)-C(46)	119.23(19)
C(42)-C(41)-C(31)	120.30(19)
C(46)-C(41)-C(31)	120.43(19)
C(41)-C(42)-C(43)	120.1(2)
C(41)-C(42)-H(42A)	120.0
C(43)-C(42)-H(42A)	120.0
C(44)-C(43)-C(42)	120.2(2)
C(44)-C(43)-H(43A)	119.9
C(42)-C(43)-H(43A)	119.9
C(43)-C(44)-C(45)	120.2(2)
C(43)-C(44)-H(44A)	119.9
C(45)-C(44)-H(44A)	119.9
C(44)-C(45)-C(46)	120.2(2)
C(44)-C(45)-H(45A)	119.9
C(46)-C(45)-H(45A)	119.9
C(45)-C(46)-C(41)	120.0(2)
C(45)-C(46)-H(46A)	120.0
C(41)-C(46)-H(46A)	120.0
C(52)-C(47)-C(48)	119.5(2)
C(52)-C(47)-C(32)	119.6(2)
C(48)-C(47)-C(32)	120.3(2)
C(47)-C(48)-C(49)	119.4(2)
C(47)-C(48)-H(48A)	120.3
C(49)-C(48)-H(48A)	120.3
C(50)-C(49)-C(48)	120.5(3)
C(50)-C(49)-H(49A)	119.7
C(48)-C(49)-H(49A)	119.7
C(49)-C(50)-C(51)	120.3(2)
C(49)-C(50)-H(50A)	119.9

C(51)-C(50)-H(50A)	119.9
C(52)-C(51)-C(50)	119.3(2)
C(52)-C(51)-H(51A)	120.4
C(50)-C(51)-H(51A)	120.4
C(51)-C(52)-C(47)	121.0(2)
C(51)-C(52)-H(52A)	119.5
C(47)-C(52)-H(52A)	119.5
C(54)-C(53)-C(40)	125.10(19)
C(54)-C(53)-S(3)	111.59(16)
C(40)-C(53)-S(3)	122.21(16)
C(53)-C(54)-C(55)	108.7(2)
C(53)-C(54)-H(54A)	125.6
C(55)-C(54)-H(54A)	125.6
C(56)-C(55)-C(54)	114.5(2)
C(56)-C(55)-H(55A)	122.8
C(54)-C(55)-H(55A)	122.8
C(55)-C(56)-S(3)	112.86(18)
C(55)-C(56)-H(56A)	123.6
S(3)-C(56)-H(56A)	123.6
C(58)-C(57)-C(39)	130.6(2)
C(58)-C(57)-S(4)	111.63(17)
C(39)-C(57)-S(4)	117.49(17)
C(57)-C(58)-C(59)	112.0(2)
C(57)-C(58)-H(58A)	124.0
C(59)-C(58)-H(58A)	124.0
C(60)-C(59)-C(58)	112.4(2)
C(60)-C(59)-H(59A)	123.8
C(58)-C(59)-H(59A)	123.8
C(59)-C(60)-S(4)	112.60(18)
C(59)-C(60)-H(60A)	123.7
S(4)-C(60)-H(60A)	123.7
C(1)-N(1)-C(4)	117.97(17)
C(1)-N(1)-Cu(1)	131.90(14)
C(4)-N(1)-Cu(1)	109.93(13)
C(10)-N(2)-C(5)	118.52(18)
C(10)-N(2)-Cu(1)	130.45(14)

C(5)-N(2)-Cu(1)	110.37(14)
C(31)-N(3)-C(34)	117.66(18)
C(31)-N(3)-Cu(1)	133.53(14)
C(34)-N(3)-Cu(1)	107.69(13)
C(40)-N(4)-C(35)	117.60(17)
C(40)-N(4)-Cu(1)	132.78(15)
C(35)-N(4)-Cu(1)	109.61(13)
C(2)-N(5)-C(3)	118.43(18)
C(9)-N(6)-C(6)	118.01(18)
C(32)-N(7)-C(33)	117.88(19)
C(39)-N(8)-C(36)	118.10(18)
F(2)-P(1)-F(2)#1	180.0
F(2)-P(1)-F(3)	90.06(8)
F(2)#1-P(1)-F(3)	89.94(8)
F(2)-P(1)-F(3)#1	89.94(8)
F(2)#1-P(1)-F(3)#1	90.06(8)
F(3)-P(1)-F(3)#1	180.0
F(2)-P(1)-F(1)#1	89.98(8)
F(2)#1-P(1)-F(1)#1	90.02(8)
F(3)-P(1)-F(1)#1	89.99(8)
F(3)#1-P(1)-F(1)#1	90.01(8)
F(2)-P(1)-F(1)	90.02(8)
F(2)#1-P(1)-F(1)	89.98(8)
F(3)-P(1)-F(1)	90.01(8)
F(3)#1-P(1)-F(1)	89.99(8)
F(1)#1-P(1)-F(1)	180.0
F(5)#2-P(2)-F(5)	180.0
F(5)#2-P(2)-F(4)	90.11(7)
F(5)-P(2)-F(4)	89.89(7)
F(5)#2-P(2)-F(4)#2	89.89(7)
F(5)-P(2)-F(4)#2	90.11(7)
F(4)-P(2)-F(4)#2	180.00(11)
F(5)#2-P(2)-F(6)#2	90.02(7)
F(5)-P(2)-F(6)#2	89.98(7)
F(4)-P(2)-F(6)#2	89.99(7)
F(4)#2-P(2)-F(6)#2	90.01(7)

F(5)#2-P(2)-F(6)	89.98(7)
F(5)-P(2)-F(6)	90.02(7)
F(4)-P(2)-F(6)	90.01(7)
F(4)#2-P(2)-F(6)	89.99(7)
F(6)#2-P(2)-F(6)	179.999(2)
C(26)-S(1)-C(23)	92.15(12)
C(30)-S(2)-C(27)	92.17(12)
C(56)-S(3)-C(53)	92.33(11)
C(60)-S(4)-C(57)	91.39(12)
N(4)-Cu(1)-N(1)	135.62(7)
N(4)-Cu(1)-N(2)	130.03(7)
N(1)-Cu(1)-N(2)	82.51(7)
N(4)-Cu(1)-N(3)	84.40(7)
N(1)-Cu(1)-N(3)	122.16(7)
N(2)-Cu(1)-N(3)	101.56(7)

Symmetry transformations used to generate equivalent atoms:

#1 $-x, -y+2, -z$ #2 $-x+1, -y, -z+1$

Table 3. Torsion angles [°] for a.

N(1)-C(1)-C(2)-N(5)	3.8(3)
C(11)-C(1)-C(2)-N(5)	-172.8(2)
N(1)-C(1)-C(2)-C(17)	-177.39(19)
C(11)-C(1)-C(2)-C(17)	6.0(3)
N(5)-C(3)-C(4)-N(1)	0.8(3)
C(8)-C(3)-C(4)-N(1)	178.84(18)
N(5)-C(3)-C(4)-C(5)	-179.25(18)
C(8)-C(3)-C(4)-C(5)	-1.3(3)
N(1)-C(4)-C(5)-N(2)	-1.0(3)
C(3)-C(4)-C(5)-N(2)	179.09(18)
N(1)-C(4)-C(5)-C(6)	-178.88(18)
C(3)-C(4)-C(5)-C(6)	1.2(3)
N(2)-C(5)-C(6)-N(6)	2.4(3)
C(4)-C(5)-C(6)-N(6)	-179.77(18)
N(2)-C(5)-C(6)-C(7)	-178.12(19)
C(4)-C(5)-C(6)-C(7)	-0.3(3)
N(6)-C(6)-C(7)-C(8)	178.9(2)
C(5)-C(6)-C(7)-C(8)	-0.5(3)
C(6)-C(7)-C(8)-C(3)	0.4(3)
N(5)-C(3)-C(8)-C(7)	178.4(2)
C(4)-C(3)-C(8)-C(7)	0.5(3)
N(6)-C(9)-C(10)-N(2)	2.8(3)
C(27)-C(9)-C(10)-N(2)	-176.21(19)
N(6)-C(9)-C(10)-C(23)	-176.94(19)
C(27)-C(9)-C(10)-C(23)	4.0(3)
N(1)-C(1)-C(11)-C(12)	62.8(3)
C(2)-C(1)-C(11)-C(12)	-120.4(2)
N(1)-C(1)-C(11)-C(16)	-112.7(2)
C(2)-C(1)-C(11)-C(16)	64.1(3)
C(16)-C(11)-C(12)-C(13)	-1.2(3)
C(1)-C(11)-C(12)-C(13)	-176.8(2)
C(11)-C(12)-C(13)-C(14)	1.4(4)
C(12)-C(13)-C(14)-C(15)	0.1(4)
C(13)-C(14)-C(15)-C(16)	-1.9(4)

C(14)-C(15)-C(16)-C(11)	2.1(4)
C(12)-C(11)-C(16)-C(15)	-0.5(3)
C(1)-C(11)-C(16)-C(15)	175.1(2)
N(5)-C(2)-C(17)-C(18)	-153.2(2)
C(1)-C(2)-C(17)-C(18)	28.0(3)
N(5)-C(2)-C(17)-C(22)	25.1(3)
C(1)-C(2)-C(17)-C(22)	-153.7(2)
C(22)-C(17)-C(18)-C(19)	2.2(3)
C(2)-C(17)-C(18)-C(19)	-179.5(2)
C(17)-C(18)-C(19)-C(20)	0.6(4)
C(18)-C(19)-C(20)-C(21)	-2.1(4)
C(19)-C(20)-C(21)-C(22)	0.7(4)
C(20)-C(21)-C(22)-C(17)	2.3(4)
C(18)-C(17)-C(22)-C(21)	-3.7(3)
C(2)-C(17)-C(22)-C(21)	177.9(2)
N(2)-C(10)-C(23)-C(24)	65.1(3)
C(9)-C(10)-C(23)-C(24)	-115.1(3)
N(2)-C(10)-C(23)-S(1)	-109.5(2)
C(9)-C(10)-C(23)-S(1)	70.3(3)
C(10)-C(23)-C(24)-C(25)	-175.7(2)
S(1)-C(23)-C(24)-C(25)	-0.7(2)
C(23)-C(24)-C(25)-C(26)	0.2(3)
C(24)-C(25)-C(26)-S(1)	0.4(3)
N(6)-C(9)-C(27)-C(28)	-165.0(2)
C(10)-C(9)-C(27)-C(28)	14.1(4)
N(6)-C(9)-C(27)-S(2)	11.2(3)
C(10)-C(9)-C(27)-S(2)	-169.65(16)
C(9)-C(27)-C(28)-C(29)	178.2(2)
S(2)-C(27)-C(28)-C(29)	1.8(3)
C(27)-C(28)-C(29)-C(30)	-0.3(3)
C(28)-C(29)-C(30)-S(2)	-1.2(3)
N(3)-C(31)-C(32)-N(7)	1.1(3)
C(41)-C(31)-C(32)-N(7)	-176.4(2)
N(3)-C(31)-C(32)-C(47)	-178.1(2)
C(41)-C(31)-C(32)-C(47)	4.4(3)
N(7)-C(33)-C(34)-N(3)	-0.4(3)

C(38)-C(33)-C(34)-N(3)	179.5(2)
N(7)-C(33)-C(34)-C(35)	174.8(2)
C(38)-C(33)-C(34)-C(35)	-5.3(3)
N(3)-C(34)-C(35)-N(4)	7.8(3)
C(33)-C(34)-C(35)-N(4)	-167.55(19)
N(3)-C(34)-C(35)-C(36)	-179.62(19)
C(33)-C(34)-C(35)-C(36)	5.1(3)
N(4)-C(35)-C(36)-N(8)	-10.1(3)
C(34)-C(35)-C(36)-N(8)	177.5(2)
N(4)-C(35)-C(36)-C(37)	171.3(2)
C(34)-C(35)-C(36)-C(37)	-1.2(3)
N(8)-C(36)-C(37)-C(38)	178.7(2)
C(35)-C(36)-C(37)-C(38)	-2.6(4)
C(36)-C(37)-C(38)-C(33)	2.4(4)
N(7)-C(33)-C(38)-C(37)	-178.5(2)
C(34)-C(33)-C(38)-C(37)	1.6(4)
N(8)-C(39)-C(40)-N(4)	-13.7(3)
C(57)-C(39)-C(40)-N(4)	165.9(2)
N(8)-C(39)-C(40)-C(53)	159.5(2)
C(57)-C(39)-C(40)-C(53)	-20.9(3)
N(3)-C(31)-C(41)-C(42)	60.1(3)
C(32)-C(31)-C(41)-C(42)	-122.3(2)
N(3)-C(31)-C(41)-C(46)	-117.7(2)
C(32)-C(31)-C(41)-C(46)	59.9(3)
C(46)-C(41)-C(42)-C(43)	0.1(3)
C(31)-C(41)-C(42)-C(43)	-177.64(19)
C(41)-C(42)-C(43)-C(44)	1.4(3)
C(42)-C(43)-C(44)-C(45)	-1.5(3)
C(43)-C(44)-C(45)-C(46)	0.1(4)
C(44)-C(45)-C(46)-C(41)	1.4(3)
C(42)-C(41)-C(46)-C(45)	-1.5(3)
C(31)-C(41)-C(46)-C(45)	176.3(2)
N(7)-C(32)-C(47)-C(52)	65.9(3)
C(31)-C(32)-C(47)-C(52)	-114.8(2)
N(7)-C(32)-C(47)-C(48)	-105.5(2)
C(31)-C(32)-C(47)-C(48)	73.7(3)

C(52)-C(47)-C(48)-C(49)	-1.1(3)
C(32)-C(47)-C(48)-C(49)	170.4(2)
C(47)-C(48)-C(49)-C(50)	1.6(4)
C(48)-C(49)-C(50)-C(51)	-0.5(4)
C(49)-C(50)-C(51)-C(52)	-1.1(4)
C(50)-C(51)-C(52)-C(47)	1.6(4)
C(48)-C(47)-C(52)-C(51)	-0.5(3)
C(32)-C(47)-C(52)-C(51)	-172.0(2)
N(4)-C(40)-C(53)-C(54)	141.5(2)
C(39)-C(40)-C(53)-C(54)	-31.8(3)
N(4)-C(40)-C(53)-S(3)	-25.5(3)
C(39)-C(40)-C(53)-S(3)	161.19(17)
C(40)-C(53)-C(54)-C(55)	-170.1(2)
S(3)-C(53)-C(54)-C(55)	-1.9(2)
C(53)-C(54)-C(55)-C(56)	1.7(3)
C(54)-C(55)-C(56)-S(3)	-0.7(3)
N(8)-C(39)-C(57)-C(58)	147.3(3)
C(40)-C(39)-C(57)-C(58)	-32.3(4)
N(8)-C(39)-C(57)-S(4)	-25.6(3)
C(40)-C(39)-C(57)-S(4)	154.78(19)
C(39)-C(57)-C(58)-C(59)	-174.0(3)
S(4)-C(57)-C(58)-C(59)	-0.7(3)
C(57)-C(58)-C(59)-C(60)	-0.2(3)
C(58)-C(59)-C(60)-S(4)	1.1(3)
C(2)-C(1)-N(1)-C(4)	-6.0(3)
C(11)-C(1)-N(1)-C(4)	171.03(18)
C(2)-C(1)-N(1)-Cu(1)	168.31(15)
C(11)-C(1)-N(1)-Cu(1)	-14.7(3)
C(3)-C(4)-N(1)-C(1)	3.8(3)
C(5)-C(4)-N(1)-C(1)	-176.12(18)
C(3)-C(4)-N(1)-Cu(1)	-171.69(16)
C(5)-C(4)-N(1)-Cu(1)	8.4(2)
C(9)-C(10)-N(2)-C(5)	-1.8(3)
C(23)-C(10)-N(2)-C(5)	178.02(18)
C(9)-C(10)-N(2)-Cu(1)	-171.45(14)
C(23)-C(10)-N(2)-Cu(1)	8.4(3)

C(6)-C(5)-N(2)-C(10)	-0.8(3)
C(4)-C(5)-N(2)-C(10)	-178.61(18)
C(6)-C(5)-N(2)-Cu(1)	170.87(16)
C(4)-C(5)-N(2)-Cu(1)	-7.0(2)
C(32)-C(31)-N(3)-C(34)	-0.4(3)
C(41)-C(31)-N(3)-C(34)	177.30(18)
C(32)-C(31)-N(3)-Cu(1)	-166.52(15)
C(41)-C(31)-N(3)-Cu(1)	11.1(3)
C(33)-C(34)-N(3)-C(31)	0.0(3)
C(35)-C(34)-N(3)-C(31)	-175.15(19)
C(33)-C(34)-N(3)-Cu(1)	169.56(17)
C(35)-C(34)-N(3)-Cu(1)	-5.6(2)
C(39)-C(40)-N(4)-C(35)	9.9(3)
C(53)-C(40)-N(4)-C(35)	-163.61(19)
C(39)-C(40)-N(4)-Cu(1)	-171.46(15)
C(53)-C(40)-N(4)-Cu(1)	15.1(3)
C(36)-C(35)-N(4)-C(40)	1.3(3)
C(34)-C(35)-N(4)-C(40)	173.77(19)
C(36)-C(35)-N(4)-Cu(1)	-177.64(17)
C(34)-C(35)-N(4)-Cu(1)	-5.2(2)
C(1)-C(2)-N(5)-C(3)	0.8(3)
C(17)-C(2)-N(5)-C(3)	-178.03(18)
C(4)-C(3)-N(5)-C(2)	-3.1(3)
C(8)-C(3)-N(5)-C(2)	178.96(19)
C(10)-C(9)-N(6)-C(6)	-1.2(3)
C(27)-C(9)-N(6)-C(6)	177.96(18)
C(5)-C(6)-N(6)-C(9)	-1.4(3)
C(7)-C(6)-N(6)-C(9)	179.20(19)
C(31)-C(32)-N(7)-C(33)	-1.4(3)
C(47)-C(32)-N(7)-C(33)	177.8(2)
C(34)-C(33)-N(7)-C(32)	1.1(3)
C(38)-C(33)-N(7)-C(32)	-178.8(2)
C(40)-C(39)-N(8)-C(36)	5.0(3)
C(57)-C(39)-N(8)-C(36)	-174.6(2)
C(35)-C(36)-N(8)-C(39)	6.4(3)
C(37)-C(36)-N(8)-C(39)	-174.9(2)

C(25)-C(26)-S(1)-C(23)	-0.7(2)
C(24)-C(23)-S(1)-C(26)	0.82(18)
C(10)-C(23)-S(1)-C(26)	176.16(19)
C(29)-C(30)-S(2)-C(27)	1.9(2)
C(28)-C(27)-S(2)-C(30)	-2.07(19)
C(9)-C(27)-S(2)-C(30)	-179.07(18)
C(55)-C(56)-S(3)-C(53)	-0.43(19)
C(54)-C(53)-S(3)-C(56)	1.39(17)
C(40)-C(53)-S(3)-C(56)	170.01(19)
C(59)-C(60)-S(4)-C(57)	-1.3(2)
C(58)-C(57)-S(4)-C(60)	1.1(2)
C(39)-C(57)-S(4)-C(60)	175.3(2)
C(40)-N(4)-Cu(1)-N(1)	51.2(2)
C(35)-N(4)-Cu(1)-N(1)	-130.08(14)
C(40)-N(4)-Cu(1)-N(2)	-76.8(2)
C(35)-N(4)-Cu(1)-N(2)	101.97(15)
C(40)-N(4)-Cu(1)-N(3)	-177.2(2)
C(35)-N(4)-Cu(1)-N(3)	1.56(14)
C(1)-N(1)-Cu(1)-N(4)	33.6(2)
C(4)-N(1)-Cu(1)-N(4)	-151.75(13)
C(1)-N(1)-Cu(1)-N(2)	176.12(19)
C(4)-N(1)-Cu(1)-N(2)	-9.26(13)
C(1)-N(1)-Cu(1)-N(3)	-84.90(19)
C(4)-N(1)-Cu(1)-N(3)	89.73(14)
C(10)-N(2)-Cu(1)-N(4)	-34.7(2)
C(5)-N(2)-Cu(1)-N(4)	155.03(13)
C(10)-N(2)-Cu(1)-N(1)	179.14(19)
C(5)-N(2)-Cu(1)-N(1)	8.83(13)
C(10)-N(2)-Cu(1)-N(3)	57.74(19)
C(5)-N(2)-Cu(1)-N(3)	-112.58(14)
C(31)-N(3)-Cu(1)-N(4)	169.3(2)
C(34)-N(3)-Cu(1)-N(4)	2.16(13)
C(31)-N(3)-Cu(1)-N(1)	-48.8(2)
C(34)-N(3)-Cu(1)-N(1)	144.03(13)
C(31)-N(3)-Cu(1)-N(2)	39.5(2)
C(34)-N(3)-Cu(1)-N(2)	-127.60(13)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z #2 -x+1,-y,-z+1

Table 1. Crystal data and structure refinement for **Complex 3**.

Identification code	Complex 3	
Empirical formula	C ₆₈ H ₄₀ Cu F ₁₀ N ₈ P	
Formula weight	1253.59	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	?	
Space group	?	
Unit cell dimensions	a = 11.1088(4) Å	α = 105.045(3)°.
	b = 15.1156(5) Å	β = 99.568(3)°.
	c = 18.2193(6) Å	γ = 104.833(3)°.
Volume	2765.87(16) Å ³	
Z	2	
Density (calculated)	1.505 Mg/m ³	
Absorption coefficient	1.580 mm ⁻¹	
F(000)	1276	
Crystal size	0.35 x 0.18 x 0.10 mm ³	
Theta range for data collection	3.41 to 72.50°.	
Index ranges	-13<=h<=13, -18<=k<=18, -22<=l<=22	
Reflections collected	17841	
Independent reflections	17841 [R(int) = 0.0000]	
Completeness to theta = 72.50°	98.9 %	
Max. and min. transmission	0.8580 and 0.6078	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	17841 / 0 / 794	
Goodness-of-fit on F ²	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0673, wR2 = 0.1846	
R indices (all data)	R1 = 0.0759, wR2 = 0.1959	
Largest diff. peak and hole	2.219 and -0.742 e.Å ⁻³	

Table 2. Bond lengths [\AA] and angles [$^\circ$] for a.

C(1)-N(1)	1.338(4)
C(1)-C(2)	1.432(4)
C(1)-C(11)	1.487(4)
C(2)-N(5)	1.330(4)
C(2)-C(17)	1.482(4)
C(3)-N(5)	1.356(4)
C(3)-C(4)	1.397(4)
C(3)-C(8)	1.437(4)
C(4)-N(1)	1.348(4)
C(4)-C(5)	1.425(4)
C(5)-N(2)	1.360(3)
C(5)-C(6)	1.403(4)
C(6)-N(6)	1.356(4)
C(6)-C(7)	1.432(4)
C(7)-C(8)	1.354(5)
C(7)-H(7A)	0.9500
C(8)-H(8A)	0.9500
C(9)-N(6)	1.332(4)
C(9)-C(10)	1.434(4)
C(9)-C(29)	1.493(4)
C(10)-N(2)	1.328(4)
C(10)-C(23)	1.487(4)
C(11)-C(12)	1.390(4)
C(11)-C(16)	1.391(4)
C(12)-C(13)	1.377(4)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.387(5)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.390(5)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.388(4)
C(15)-H(15A)	0.9500
C(16)-H(16A)	0.9500
C(17)-C(18)	1.393(5)

C(17)-C(22)	1.395(5)
C(18)-C(19)	1.385(5)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.386(6)
C(19)-H(19A)	0.9500
C(20)-C(21)	1.389(6)
C(20)-H(20A)	0.9500
C(21)-C(22)	1.389(5)
C(21)-H(21A)	0.9500
C(22)-H(22A)	0.9500
C(23)-C(28)	1.392(4)
C(23)-C(24)	1.397(4)
C(24)-C(25)	1.384(4)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.379(4)
C(25)-H(25A)	0.9500
C(26)-F(1)	1.349(3)
C(26)-C(27)	1.370(4)
C(27)-C(28)	1.398(4)
C(27)-H(27A)	0.9500
C(28)-H(28A)	0.9500
C(29)-C(34)	1.383(4)
C(29)-C(30)	1.391(4)
C(30)-C(31)	1.395(5)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.370(5)
C(31)-H(31A)	0.9500
C(32)-F(2)	1.337(4)
C(32)-C(33)	1.371(5)
C(33)-C(34)	1.396(4)
C(33)-H(33A)	0.9500
C(34)-H(34A)	0.9500
C(35)-N(3)	1.331(4)
C(35)-C(36)	1.436(4)
C(35)-C(45)	1.474(4)
C(36)-N(7)	1.332(4)

C(36)-C(51)	1.483(4)
C(37)-N(7)	1.361(4)
C(37)-C(38)	1.397(4)
C(37)-C(42)	1.431(4)
C(38)-N(3)	1.364(3)
C(38)-C(39)	1.429(4)
C(39)-N(4)	1.363(4)
C(39)-C(40)	1.393(4)
C(40)-N(8)	1.366(4)
C(40)-C(41)	1.428(4)
C(41)-C(42)	1.353(4)
C(41)-H(41A)	0.9500
C(42)-H(42A)	0.9500
C(43)-N(8)	1.318(4)
C(43)-C(44)	1.429(4)
C(43)-C(63)	1.489(4)
C(44)-N(4)	1.328(4)
C(44)-C(57)	1.484(4)
C(45)-C(46)	1.382(4)
C(45)-C(50)	1.403(4)
C(46)-C(47)	1.396(4)
C(46)-H(46A)	0.9500
C(47)-C(48)	1.389(5)
C(47)-H(47A)	0.9500
C(48)-C(49)	1.379(5)
C(48)-H(48A)	0.9500
C(49)-C(50)	1.391(5)
C(49)-H(49A)	0.9500
C(50)-H(50A)	0.9500
C(51)-C(52)	1.387(4)
C(51)-C(56)	1.388(4)
C(52)-C(53)	1.385(4)
C(52)-H(52A)	0.9500
C(53)-C(54)	1.394(5)
C(53)-H(53A)	0.9500
C(54)-C(55)	1.388(5)

C(54)-H(54A)	0.9500
C(55)-C(56)	1.383(5)
C(55)-H(55A)	0.9500
C(56)-H(56A)	0.9500
C(57)-C(58)	1.399(4)
C(57)-C(62)	1.400(4)
C(58)-C(59)	1.374(4)
C(58)-H(58A)	0.9500
C(59)-C(60)	1.376(4)
C(59)-H(59A)	0.9500
C(60)-F(3)	1.331(3)
C(60)-C(61)	1.376(4)
C(61)-C(62)	1.387(4)
C(61)-H(61A)	0.9500
C(62)-H(62A)	0.9500
C(63)-C(64)	1.389(4)
C(63)-C(68)	1.390(4)
C(64)-C(65)	1.386(4)
C(64)-H(64A)	0.9500
C(65)-C(66)	1.370(6)
C(65)-H(65A)	0.9500
C(66)-F(4)	1.321(4)
C(66)-C(67)	1.386(5)
C(67)-C(68)	1.379(5)
C(67)-H(67A)	0.9500
C(68)-H(68A)	0.9500
N(1)-Cu(1)	2.055(2)
N(2)-Cu(1)	2.045(2)
N(3)-Cu(1)	2.065(2)
N(4)-Cu(1)	2.030(2)
F(5)-P(1)	1.6064(19)
F(6)-P(1)	1.5882(19)
F(7)-P(1)	1.6043(18)
F(8)-P(1)	1.6038(18)
F(9)-P(1)	1.6023(18)
F(10)-P(1)	1.6087(18)

N(1)-C(1)-C(2)	119.5(3)
N(1)-C(1)-C(11)	115.4(2)
C(2)-C(1)-C(11)	125.0(3)
N(5)-C(2)-C(1)	122.0(3)
N(5)-C(2)-C(17)	116.3(3)
C(1)-C(2)-C(17)	121.7(3)
N(5)-C(3)-C(4)	120.7(3)
N(5)-C(3)-C(8)	119.8(3)
C(4)-C(3)-C(8)	119.5(3)
N(1)-C(4)-C(3)	121.7(3)
N(1)-C(4)-C(5)	118.1(2)
C(3)-C(4)-C(5)	120.1(3)
N(2)-C(5)-C(6)	121.5(3)
N(2)-C(5)-C(4)	118.9(2)
C(6)-C(5)-C(4)	119.6(2)
N(6)-C(6)-C(5)	120.6(3)
N(6)-C(6)-C(7)	119.9(3)
C(5)-C(6)-C(7)	119.4(3)
C(8)-C(7)-C(6)	121.0(3)
C(8)-C(7)-H(7A)	119.5
C(6)-C(7)-H(7A)	119.5
C(7)-C(8)-C(3)	120.4(3)
C(7)-C(8)-H(8A)	119.8
C(3)-C(8)-H(8A)	119.8
N(6)-C(9)-C(10)	121.7(3)
N(6)-C(9)-C(29)	115.3(2)
C(10)-C(9)-C(29)	122.9(2)
N(2)-C(10)-C(9)	120.2(2)
N(2)-C(10)-C(23)	116.8(2)
C(9)-C(10)-C(23)	122.8(2)
C(12)-C(11)-C(16)	119.7(3)
C(12)-C(11)-C(1)	119.3(3)
C(16)-C(11)-C(1)	120.7(3)
C(13)-C(12)-C(11)	120.3(3)
C(13)-C(12)-H(12A)	119.8

C(11)-C(12)-H(12A)	119.8
C(12)-C(13)-C(14)	120.3(3)
C(12)-C(13)-H(13A)	119.9
C(14)-C(13)-H(13A)	119.9
C(13)-C(14)-C(15)	119.6(3)
C(13)-C(14)-H(14A)	120.2
C(15)-C(14)-H(14A)	120.2
C(16)-C(15)-C(14)	120.4(3)
C(16)-C(15)-H(15A)	119.8
C(14)-C(15)-H(15A)	119.8
C(15)-C(16)-C(11)	119.6(3)
C(15)-C(16)-H(16A)	120.2
C(11)-C(16)-H(16A)	120.2
C(18)-C(17)-C(22)	119.9(3)
C(18)-C(17)-C(2)	121.6(3)
C(22)-C(17)-C(2)	118.5(3)
C(19)-C(18)-C(17)	119.4(3)
C(19)-C(18)-H(18A)	120.3
C(17)-C(18)-H(18A)	120.3
C(20)-C(19)-C(18)	120.9(4)
C(20)-C(19)-H(19A)	119.5
C(18)-C(19)-H(19A)	119.5
C(19)-C(20)-C(21)	119.7(3)
C(19)-C(20)-H(20A)	120.2
C(21)-C(20)-H(20A)	120.2
C(22)-C(21)-C(20)	120.0(4)
C(22)-C(21)-H(21A)	120.0
C(20)-C(21)-H(21A)	120.0
C(21)-C(22)-C(17)	120.0(4)
C(21)-C(22)-H(22A)	120.0
C(17)-C(22)-H(22A)	120.0
C(28)-C(23)-C(24)	119.3(3)
C(28)-C(23)-C(10)	121.3(2)
C(24)-C(23)-C(10)	119.4(2)
C(25)-C(24)-C(23)	120.5(3)
C(25)-C(24)-H(24A)	119.8

C(23)-C(24)-H(24A)	119.8
C(26)-C(25)-C(24)	118.3(3)
C(26)-C(25)-H(25A)	120.8
C(24)-C(25)-H(25A)	120.8
F(1)-C(26)-C(27)	118.6(3)
F(1)-C(26)-C(25)	117.9(3)
C(27)-C(26)-C(25)	123.5(3)
C(26)-C(27)-C(28)	117.6(3)
C(26)-C(27)-H(27A)	121.2
C(28)-C(27)-H(27A)	121.2
C(23)-C(28)-C(27)	120.9(3)
C(23)-C(28)-H(28A)	119.6
C(27)-C(28)-H(28A)	119.6
C(34)-C(29)-C(30)	120.2(3)
C(34)-C(29)-C(9)	120.9(3)
C(30)-C(29)-C(9)	118.7(3)
C(29)-C(30)-C(31)	120.2(3)
C(29)-C(30)-H(30A)	119.9
C(31)-C(30)-H(30A)	119.9
C(32)-C(31)-C(30)	118.0(3)
C(32)-C(31)-H(31A)	121.0
C(30)-C(31)-H(31A)	121.0
F(2)-C(32)-C(31)	117.4(3)
F(2)-C(32)-C(33)	119.4(3)
C(31)-C(32)-C(33)	123.2(3)
C(32)-C(33)-C(34)	118.4(3)
C(32)-C(33)-H(33A)	120.8
C(34)-C(33)-H(33A)	120.8
C(29)-C(34)-C(33)	119.9(3)
C(29)-C(34)-H(34A)	120.1
C(33)-C(34)-H(34A)	120.1
N(3)-C(35)-C(36)	120.0(3)
N(3)-C(35)-C(45)	117.7(2)
C(36)-C(35)-C(45)	122.2(3)
N(7)-C(36)-C(35)	121.9(3)
N(7)-C(36)-C(51)	117.3(3)

C(35)-C(36)-C(51)	120.7(3)
N(7)-C(37)-C(38)	120.7(3)
N(7)-C(37)-C(42)	119.8(3)
C(38)-C(37)-C(42)	119.5(3)
N(3)-C(38)-C(37)	121.8(3)
N(3)-C(38)-C(39)	118.3(2)
C(37)-C(38)-C(39)	119.9(2)
N(4)-C(39)-C(40)	121.8(3)
N(4)-C(39)-C(38)	118.9(2)
C(40)-C(39)-C(38)	119.3(3)
N(8)-C(40)-C(39)	120.3(3)
N(8)-C(40)-C(41)	119.4(3)
C(39)-C(40)-C(41)	120.2(3)
C(42)-C(41)-C(40)	120.3(3)
C(42)-C(41)-H(41A)	119.8
C(40)-C(41)-H(41A)	119.8
C(41)-C(42)-C(37)	120.7(3)
C(41)-C(42)-H(42A)	119.6
C(37)-C(42)-H(42A)	119.6
N(8)-C(43)-C(44)	122.3(3)
N(8)-C(43)-C(63)	115.1(2)
C(44)-C(43)-C(63)	122.6(3)
N(4)-C(44)-C(43)	120.0(3)
N(4)-C(44)-C(57)	117.9(2)
C(43)-C(44)-C(57)	122.1(3)
C(46)-C(45)-C(50)	118.9(3)
C(46)-C(45)-C(35)	121.2(3)
C(50)-C(45)-C(35)	119.8(3)
C(45)-C(46)-C(47)	120.9(3)
C(45)-C(46)-H(46A)	119.5
C(47)-C(46)-H(46A)	119.5
C(48)-C(47)-C(46)	119.5(3)
C(48)-C(47)-H(47A)	120.3
C(46)-C(47)-H(47A)	120.3
C(49)-C(48)-C(47)	120.3(3)
C(49)-C(48)-H(48A)	119.9

C(47)-C(48)-H(48A)	119.9
C(48)-C(49)-C(50)	120.1(3)
C(48)-C(49)-H(49A)	119.9
C(50)-C(49)-H(49A)	119.9
C(49)-C(50)-C(45)	120.3(3)
C(49)-C(50)-H(50A)	119.9
C(45)-C(50)-H(50A)	119.9
C(52)-C(51)-C(56)	120.0(3)
C(52)-C(51)-C(36)	120.1(3)
C(56)-C(51)-C(36)	119.9(3)
C(53)-C(52)-C(51)	120.2(3)
C(53)-C(52)-H(52A)	119.9
C(51)-C(52)-H(52A)	119.9
C(52)-C(53)-C(54)	119.8(3)
C(52)-C(53)-H(53A)	120.1
C(54)-C(53)-H(53A)	120.1
C(55)-C(54)-C(53)	119.7(3)
C(55)-C(54)-H(54A)	120.2
C(53)-C(54)-H(54A)	120.2
C(56)-C(55)-C(54)	120.5(3)
C(56)-C(55)-H(55A)	119.8
C(54)-C(55)-H(55A)	119.8
C(55)-C(56)-C(51)	119.7(3)
C(55)-C(56)-H(56A)	120.1
C(51)-C(56)-H(56A)	120.1
C(58)-C(57)-C(62)	118.7(3)
C(58)-C(57)-C(44)	120.4(2)
C(62)-C(57)-C(44)	120.9(2)
C(59)-C(58)-C(57)	120.7(3)
C(59)-C(58)-H(58A)	119.6
C(57)-C(58)-H(58A)	119.6
C(58)-C(59)-C(60)	118.8(3)
C(58)-C(59)-H(59A)	120.6
C(60)-C(59)-H(59A)	120.6
F(3)-C(60)-C(59)	118.2(3)
F(3)-C(60)-C(61)	119.0(3)

C(59)-C(60)-C(61)	122.8(3)
C(60)-C(61)-C(62)	118.0(3)
C(60)-C(61)-H(61A)	121.0
C(62)-C(61)-H(61A)	121.0
C(61)-C(62)-C(57)	120.9(3)
C(61)-C(62)-H(62A)	119.6
C(57)-C(62)-H(62A)	119.6
C(64)-C(63)-C(68)	120.0(3)
C(64)-C(63)-C(43)	119.4(3)
C(68)-C(63)-C(43)	120.6(3)
C(65)-C(64)-C(63)	120.1(3)
C(65)-C(64)-H(64A)	120.0
C(63)-C(64)-H(64A)	120.0
C(66)-C(65)-C(64)	118.8(3)
C(66)-C(65)-H(65A)	120.6
C(64)-C(65)-H(65A)	120.6
F(4)-C(66)-C(65)	119.8(3)
F(4)-C(66)-C(67)	117.7(4)
C(65)-C(66)-C(67)	122.5(3)
C(68)-C(67)-C(66)	118.4(3)
C(68)-C(67)-H(67A)	120.8
C(66)-C(67)-H(67A)	120.8
C(67)-C(68)-C(63)	120.4(3)
C(67)-C(68)-H(68A)	119.8
C(63)-C(68)-H(68A)	119.8
C(1)-N(1)-C(4)	118.4(2)
C(1)-N(1)-Cu(1)	130.23(19)
C(4)-N(1)-Cu(1)	109.91(18)
C(10)-N(2)-C(5)	118.0(2)
C(10)-N(2)-Cu(1)	132.37(19)
C(5)-N(2)-Cu(1)	109.32(18)
C(35)-N(3)-C(38)	117.7(2)
C(35)-N(3)-Cu(1)	133.11(19)
C(38)-N(3)-Cu(1)	109.07(18)
C(44)-N(4)-C(39)	117.8(2)
C(44)-N(4)-Cu(1)	132.30(19)

C(39)-N(4)-Cu(1)	109.88(18)
C(2)-N(5)-C(3)	117.7(3)
C(9)-N(6)-C(6)	117.8(2)
C(36)-N(7)-C(37)	117.4(2)
C(43)-N(8)-C(40)	117.6(2)
F(6)-P(1)-F(9)	179.57(11)
F(6)-P(1)-F(8)	90.41(11)
F(9)-P(1)-F(8)	89.62(10)
F(6)-P(1)-F(7)	89.77(11)
F(9)-P(1)-F(7)	89.80(10)
F(8)-P(1)-F(7)	89.62(10)
F(6)-P(1)-F(5)	90.19(11)
F(9)-P(1)-F(5)	89.79(10)
F(8)-P(1)-F(5)	179.38(11)
F(7)-P(1)-F(5)	90.57(10)
F(6)-P(1)-F(10)	90.44(11)
F(9)-P(1)-F(10)	89.99(10)
F(8)-P(1)-F(10)	89.68(10)
F(7)-P(1)-F(10)	179.27(11)
F(5)-P(1)-F(10)	90.13(10)
N(4)-Cu(1)-N(2)	123.85(9)
N(4)-Cu(1)-N(1)	132.55(10)
N(2)-Cu(1)-N(1)	82.98(9)
N(4)-Cu(1)-N(3)	83.77(9)
N(2)-Cu(1)-N(3)	131.67(9)
N(1)-Cu(1)-N(3)	107.71(9)

Symmetry transformations used to generate equivalent atoms:

Table 3. Torsion angles [°] for a.

N(1)-C(1)-C(2)-N(5)	2.1(4)
C(11)-C(1)-C(2)-N(5)	-174.5(3)
N(1)-C(1)-C(2)-C(17)	-178.7(3)
C(11)-C(1)-C(2)-C(17)	4.7(5)
N(5)-C(3)-C(4)-N(1)	0.2(5)
C(8)-C(3)-C(4)-N(1)	-178.2(3)
N(5)-C(3)-C(4)-C(5)	175.6(3)
C(8)-C(3)-C(4)-C(5)	-2.7(4)
N(1)-C(4)-C(5)-N(2)	0.0(4)
C(3)-C(4)-C(5)-N(2)	-175.6(3)
N(1)-C(4)-C(5)-C(6)	178.9(3)
C(3)-C(4)-C(5)-C(6)	3.3(4)
N(2)-C(5)-C(6)-N(6)	0.7(4)
C(4)-C(5)-C(6)-N(6)	-178.1(3)
N(2)-C(5)-C(6)-C(7)	177.1(3)
C(4)-C(5)-C(6)-C(7)	-1.8(4)
N(6)-C(6)-C(7)-C(8)	176.1(3)
C(5)-C(6)-C(7)-C(8)	-0.2(5)
C(6)-C(7)-C(8)-C(3)	0.8(5)
N(5)-C(3)-C(8)-C(7)	-177.6(3)
C(4)-C(3)-C(8)-C(7)	0.7(5)
N(6)-C(9)-C(10)-N(2)	4.2(4)
C(29)-C(9)-C(10)-N(2)	-172.0(3)
N(6)-C(9)-C(10)-C(23)	-171.5(3)
C(29)-C(9)-C(10)-C(23)	12.3(4)
N(1)-C(1)-C(11)-C(12)	50.3(4)
C(2)-C(1)-C(11)-C(12)	-133.0(3)
N(1)-C(1)-C(11)-C(16)	-123.8(3)
C(2)-C(1)-C(11)-C(16)	52.9(4)
C(16)-C(11)-C(12)-C(13)	1.7(5)
C(1)-C(11)-C(12)-C(13)	-172.4(3)
C(11)-C(12)-C(13)-C(14)	1.9(5)
C(12)-C(13)-C(14)-C(15)	-4.0(5)
C(13)-C(14)-C(15)-C(16)	2.5(5)

C(14)-C(15)-C(16)-C(11)	1.0(5)
C(12)-C(11)-C(16)-C(15)	-3.2(5)
C(1)-C(11)-C(16)-C(15)	170.9(3)
N(5)-C(2)-C(17)-C(18)	-134.2(3)
C(1)-C(2)-C(17)-C(18)	46.6(4)
N(5)-C(2)-C(17)-C(22)	43.7(4)
C(1)-C(2)-C(17)-C(22)	-135.5(3)
C(22)-C(17)-C(18)-C(19)	0.3(5)
C(2)-C(17)-C(18)-C(19)	178.2(3)
C(17)-C(18)-C(19)-C(20)	0.3(5)
C(18)-C(19)-C(20)-C(21)	-0.4(6)
C(19)-C(20)-C(21)-C(22)	-0.1(6)
C(20)-C(21)-C(22)-C(17)	0.8(6)
C(18)-C(17)-C(22)-C(21)	-0.9(5)
C(2)-C(17)-C(22)-C(21)	-178.8(3)
N(2)-C(10)-C(23)-C(28)	46.1(4)
C(9)-C(10)-C(23)-C(28)	-138.0(3)
N(2)-C(10)-C(23)-C(24)	-129.8(3)
C(9)-C(10)-C(23)-C(24)	46.1(4)
C(28)-C(23)-C(24)-C(25)	-2.1(4)
C(10)-C(23)-C(24)-C(25)	173.9(3)
C(23)-C(24)-C(25)-C(26)	1.0(4)
C(24)-C(25)-C(26)-F(1)	-178.1(3)
C(24)-C(25)-C(26)-C(27)	0.4(5)
F(1)-C(26)-C(27)-C(28)	177.8(3)
C(25)-C(26)-C(27)-C(28)	-0.7(5)
C(24)-C(23)-C(28)-C(27)	1.8(4)
C(10)-C(23)-C(28)-C(27)	-174.1(3)
C(26)-C(27)-C(28)-C(23)	-0.4(4)
N(6)-C(9)-C(29)-C(34)	-128.5(3)
C(10)-C(9)-C(29)-C(34)	47.9(4)
N(6)-C(9)-C(29)-C(30)	46.5(4)
C(10)-C(9)-C(29)-C(30)	-137.0(3)
C(34)-C(29)-C(30)-C(31)	-0.2(4)
C(9)-C(29)-C(30)-C(31)	-175.3(3)
C(29)-C(30)-C(31)-C(32)	2.0(5)

C(30)-C(31)-C(32)-F(2)	178.2(3)
C(30)-C(31)-C(32)-C(33)	-2.7(5)
F(2)-C(32)-C(33)-C(34)	-179.4(3)
C(31)-C(32)-C(33)-C(34)	1.6(5)
C(30)-C(29)-C(34)-C(33)	-1.0(4)
C(9)-C(29)-C(34)-C(33)	174.0(3)
C(32)-C(33)-C(34)-C(29)	0.3(5)
N(3)-C(35)-C(36)-N(7)	8.3(4)
C(45)-C(35)-C(36)-N(7)	-167.7(3)
N(3)-C(35)-C(36)-C(51)	-169.7(3)
C(45)-C(35)-C(36)-C(51)	14.3(4)
N(7)-C(37)-C(38)-N(3)	5.3(4)
C(42)-C(37)-C(38)-N(3)	-176.6(3)
N(7)-C(37)-C(38)-C(39)	-177.8(3)
C(42)-C(37)-C(38)-C(39)	0.3(4)
N(3)-C(38)-C(39)-N(4)	-1.8(4)
C(37)-C(38)-C(39)-N(4)	-178.8(3)
N(3)-C(38)-C(39)-C(40)	177.7(3)
C(37)-C(38)-C(39)-C(40)	0.7(4)
N(4)-C(39)-C(40)-N(8)	2.0(4)
C(38)-C(39)-C(40)-N(8)	-177.5(3)
N(4)-C(39)-C(40)-C(41)	178.5(3)
C(38)-C(39)-C(40)-C(41)	-1.0(4)
N(8)-C(40)-C(41)-C(42)	176.7(3)
C(39)-C(40)-C(41)-C(42)	0.2(5)
C(40)-C(41)-C(42)-C(37)	0.9(5)
N(7)-C(37)-C(42)-C(41)	177.0(3)
C(38)-C(37)-C(42)-C(41)	-1.1(5)
N(8)-C(43)-C(44)-N(4)	5.5(4)
C(63)-C(43)-C(44)-N(4)	-172.2(3)
N(8)-C(43)-C(44)-C(57)	-172.5(3)
C(63)-C(43)-C(44)-C(57)	9.9(4)
N(3)-C(35)-C(45)-C(46)	48.8(4)
C(36)-C(35)-C(45)-C(46)	-135.1(3)
N(3)-C(35)-C(45)-C(50)	-127.6(3)
C(36)-C(35)-C(45)-C(50)	48.5(4)

C(50)-C(45)-C(46)-C(47)	1.2(5)
C(35)-C(45)-C(46)-C(47)	-175.3(3)
C(45)-C(46)-C(47)-C(48)	1.7(5)
C(46)-C(47)-C(48)-C(49)	-3.1(6)
C(47)-C(48)-C(49)-C(50)	1.5(6)
C(48)-C(49)-C(50)-C(45)	1.5(6)
C(46)-C(45)-C(50)-C(49)	-2.8(5)
C(35)-C(45)-C(50)-C(49)	173.7(3)
N(7)-C(36)-C(51)-C(52)	-128.6(3)
C(35)-C(36)-C(51)-C(52)	49.5(4)
N(7)-C(36)-C(51)-C(56)	51.7(4)
C(35)-C(36)-C(51)-C(56)	-130.2(3)
C(56)-C(51)-C(52)-C(53)	0.4(5)
C(36)-C(51)-C(52)-C(53)	-179.4(3)
C(51)-C(52)-C(53)-C(54)	2.1(5)
C(52)-C(53)-C(54)-C(55)	-2.6(5)
C(53)-C(54)-C(55)-C(56)	0.6(5)
C(54)-C(55)-C(56)-C(51)	1.8(5)
C(52)-C(51)-C(56)-C(55)	-2.3(5)
C(36)-C(51)-C(56)-C(55)	177.4(3)
N(4)-C(44)-C(57)-C(58)	-137.6(3)
C(43)-C(44)-C(57)-C(58)	40.5(4)
N(4)-C(44)-C(57)-C(62)	40.5(4)
C(43)-C(44)-C(57)-C(62)	-141.5(3)
C(62)-C(57)-C(58)-C(59)	0.6(4)
C(44)-C(57)-C(58)-C(59)	178.7(3)
C(57)-C(58)-C(59)-C(60)	-1.3(4)
C(58)-C(59)-C(60)-F(3)	177.9(3)
C(58)-C(59)-C(60)-C(61)	0.7(5)
F(3)-C(60)-C(61)-C(62)	-176.7(3)
C(59)-C(60)-C(61)-C(62)	0.5(5)
C(60)-C(61)-C(62)-C(57)	-1.1(4)
C(58)-C(57)-C(62)-C(61)	0.6(4)
C(44)-C(57)-C(62)-C(61)	-177.5(3)
N(8)-C(43)-C(63)-C(64)	52.4(4)
C(44)-C(43)-C(63)-C(64)	-129.8(3)

N(8)-C(43)-C(63)-C(68)	-124.2(3)
C(44)-C(43)-C(63)-C(68)	53.6(4)
C(68)-C(63)-C(64)-C(65)	-1.2(5)
C(43)-C(63)-C(64)-C(65)	-177.8(3)
C(63)-C(64)-C(65)-C(66)	1.9(5)
C(64)-C(65)-C(66)-F(4)	176.9(3)
C(64)-C(65)-C(66)-C(67)	-1.4(6)
F(4)-C(66)-C(67)-C(68)	-178.1(4)
C(65)-C(66)-C(67)-C(68)	0.2(6)
C(66)-C(67)-C(68)-C(63)	0.5(6)
C(64)-C(63)-C(68)-C(67)	0.0(5)
C(43)-C(63)-C(68)-C(67)	176.6(3)
C(2)-C(1)-N(1)-C(4)	-2.5(4)
C(11)-C(1)-N(1)-C(4)	174.4(2)
C(2)-C(1)-N(1)-Cu(1)	-167.3(2)
C(11)-C(1)-N(1)-Cu(1)	9.6(4)
C(3)-C(4)-N(1)-C(1)	1.4(4)
C(5)-C(4)-N(1)-C(1)	-174.1(3)
C(3)-C(4)-N(1)-Cu(1)	169.2(2)
C(5)-C(4)-N(1)-Cu(1)	-6.4(3)
C(9)-C(10)-N(2)-C(5)	-4.7(4)
C(23)-C(10)-N(2)-C(5)	171.4(2)
C(9)-C(10)-N(2)-Cu(1)	168.7(2)
C(23)-C(10)-N(2)-Cu(1)	-15.3(4)
C(6)-C(5)-N(2)-C(10)	2.3(4)
C(4)-C(5)-N(2)-C(10)	-178.8(2)
C(6)-C(5)-N(2)-Cu(1)	-172.5(2)
C(4)-C(5)-N(2)-Cu(1)	6.4(3)
C(36)-C(35)-N(3)-C(38)	-6.3(4)
C(45)-C(35)-N(3)-C(38)	169.9(2)
C(36)-C(35)-N(3)-Cu(1)	178.3(2)
C(45)-C(35)-N(3)-Cu(1)	-5.5(4)
C(37)-C(38)-N(3)-C(35)	-0.1(4)
C(39)-C(38)-N(3)-C(35)	-177.1(3)
C(37)-C(38)-N(3)-Cu(1)	176.3(2)
C(39)-C(38)-N(3)-Cu(1)	-0.6(3)

C(43)-C(44)-N(4)-C(39)	-5.0(4)
C(57)-C(44)-N(4)-C(39)	173.1(2)
C(43)-C(44)-N(4)-Cu(1)	172.2(2)
C(57)-C(44)-N(4)-Cu(1)	-9.7(4)
C(40)-C(39)-N(4)-C(44)	1.5(4)
C(38)-C(39)-N(4)-C(44)	-179.0(2)
C(40)-C(39)-N(4)-Cu(1)	-176.4(2)
C(38)-C(39)-N(4)-Cu(1)	3.1(3)
C(1)-C(2)-N(5)-C(3)	-0.5(4)
C(17)-C(2)-N(5)-C(3)	-179.7(3)
C(4)-C(3)-N(5)-C(2)	-0.6(4)
C(8)-C(3)-N(5)-C(2)	177.7(3)
C(10)-C(9)-N(6)-C(6)	-1.1(4)
C(29)-C(9)-N(6)-C(6)	175.4(3)
C(5)-C(6)-N(6)-C(9)	-1.3(4)
C(7)-C(6)-N(6)-C(9)	-177.6(3)
C(35)-C(36)-N(7)-C(37)	-3.2(4)
C(51)-C(36)-N(7)-C(37)	175.0(3)
C(38)-C(37)-N(7)-C(36)	-3.4(4)
C(42)-C(37)-N(7)-C(36)	178.5(3)
C(44)-C(43)-N(8)-C(40)	-1.9(4)
C(63)-C(43)-N(8)-C(40)	175.9(3)
C(39)-C(40)-N(8)-C(43)	-1.7(4)
C(41)-C(40)-N(8)-C(43)	-178.2(3)
C(44)-N(4)-Cu(1)-N(2)	42.9(3)
C(39)-N(4)-Cu(1)-N(2)	-139.69(18)
C(44)-N(4)-Cu(1)-N(1)	-71.7(3)
C(39)-N(4)-Cu(1)-N(1)	105.7(2)
C(44)-N(4)-Cu(1)-N(3)	179.9(3)
C(39)-N(4)-Cu(1)-N(3)	-2.64(18)
C(10)-N(2)-Cu(1)-N(4)	41.2(3)
C(5)-N(2)-Cu(1)-N(4)	-145.01(17)
C(10)-N(2)-Cu(1)-N(1)	178.8(3)
C(5)-N(2)-Cu(1)-N(1)	-7.46(18)
C(10)-N(2)-Cu(1)-N(3)	-73.7(3)
C(5)-N(2)-Cu(1)-N(3)	100.0(2)

C(1)-N(1)-Cu(1)-N(4)	-56.2(3)
C(4)-N(1)-Cu(1)-N(4)	137.99(18)
C(1)-N(1)-Cu(1)-N(2)	173.4(3)
C(4)-N(1)-Cu(1)-N(2)	7.54(19)
C(1)-N(1)-Cu(1)-N(3)	41.8(3)
C(4)-N(1)-Cu(1)-N(3)	-124.06(19)
C(35)-N(3)-Cu(1)-N(4)	177.5(3)
C(38)-N(3)-Cu(1)-N(4)	1.78(18)
C(35)-N(3)-Cu(1)-N(2)	-51.8(3)
C(38)-N(3)-Cu(1)-N(2)	132.53(18)
C(35)-N(3)-Cu(1)-N(1)	44.7(3)
C(38)-N(3)-Cu(1)-N(1)	-131.01(18)

Symmetry transformations used to generate equivalent atoms: