Inorganic Chemistry
including bioinorganic chemistry
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Table 1S. Details of data collection and structure refinement for Cu(I) Polymer.

Formula	C20 H17 Cl Cu N P
fw	401.33
cryst syst	monoclinic
space group	P21/N
cryst color	red
cryst habit	parallelipiped
a, Å	13.090(7)
b, Å	8.831(4)
c, Å	16.273(9)
β, deg	94.35(2)
Z	4
V, $Å^3$	1876(2)
ρ(calcd), g cm^{-3}	1.421
radiation, λ	Mo k_α 0.71073
abs coeff(μ), cm^{-1}	13.95
F(000), e	820
temp, C	-142
diffractometer	Picker (Crystal Logic)
scan mode, speed(deg/min)	θ-2θ, 6.0
2θ range, deg	2.6 - 50.0
total data collcd, unique data used	2910, 2029(I> 3σ(I))
no. of parms refined	218
final shift/error, max and avg	0.016, 0.002
max resid density, $e/Å^3$	0.59
$R = \Sigma\|\|F_o\|-\|F_c\|\|/\Sigma\|F_o\|$	0.026
$R_w = (\Sigma w(\|F_o\|-\|F_c\|)^2/\Sigma w(\|F_o\|)^2)^{1/2}$	0.034
$GOF = (\Sigma w(\|F_o\|-\|F_c\|)^2/ (No-Nv))^{1/2}$	1.235

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Table 2S. Fractional atomic coordinates and equivalent isotropic thermal parameters($Å^2$) with e.s.d.'s of the refined parameters in parenthesis for Cu(I) Polymer.

Atom	x	y	z	$U_{eq}x10^3$
Cu	0.9218(1)	0.1283(1)	0.0025(1)	25(1)
Cl	0.9987(1)	0.0194(1)	-0.1116(1)	26(1)
P	0.7572(1)	0.0766(1)	-0.0044(1)	21(1)
N	0.9727(2)	0.3472(3)	0.0038(1)	24(2)
C1	0.6835(2)	0.1343(3)	-0.0987(2)	24(2)
C2	0.5917(2)	0.0662(4)	-0.1264(2)	32(2)
C3	0.5377(3)	0.1151(5)	-0.1981(2)	42(2)
C4	0.5749(3)	0.2335(4)	-0.2419(2)	47(2)
C5	0.6659(3)	0.3019(4)	-0.2150(2)	50(3)
C6	0.7208(3)	0.2509(4)	-0.1445(2)	36(2)
C7	0.7301(2)	-0.1259(3)	-0.0014(2)	23(2)
C8	0.7716(2)	-0.2132(4)	-0.0615(2)	30(2)
C9	0.7518(3)	-0.3680(4)	-0.0656(2)	37(2)
C10	0.6934(3)	-0.4358(4)	-0.0086(2)	38(2)
C11	0.6532(3)	-0.3493(4)	0.0518(2)	38(2)
C12	0.6711(2)	-0.1939(4)	0.0557(2)	30(2)
C13	0.6896(2)	0.1560(3)	0.0797(2)	24(2)
C14	0.5930(2)	0.2226(4)	0.0692(2)	28(2)
C15	0.5495(3)	0.2884(4)	0.1361(2)	37(2)
C16	0.6012(3)	0.2872(4)	0.2125(2)	46(3)
C17	0.6960(3)	0.2200(5)	0.2236(2)	51(3)
C18	0.7412(3)	0.1549(4)	0.1578(2)	35(2)
C19	0.9483(2)	0.4465(3)	0.0611(2)	26(2)
C20	1.0248(2)	0.4024(4)	-0.0574(2)	28(2)

$$U_{eq}=[1/(6\pi^2)]x\Sigma_i\Sigma_j\beta_{ij}a_i.a_j$$

Table 3S. Anisotropic temperature factors for Cu(I) Polymer.

Atom	$U11x10^3$	$U22x10^3$	$U33x10^3$	$U12x10^3$	$U13x10^3$	$U_{23}x10^3$
Cu	28(1)	17(1)	30(1)	-6(1)	8(1)	-1(1)
Cl	37(1)	21(1)	21(1)	-3(1)	8(1)	0(1)
P	27(1)	17(1)	20(1)	-4(1)	5(1)	0(1)
N	26(2)	19(2)	26(2)	-2(1)	2(1)	2(1)
C1	36(2)	16(2)	22(2)	-1(1)	7(1)	-2(1)
C2	38(2)	34(2)	26(2)	-7(2)	2(1)	9(2)
C3	43(2)	49(2)	32(2)	1(2)	-3(2)	2(2)
C4	74(3)	37(2)	27(2)	5(2)	-5(2)	6(2)
C5	93(3)	27(2)	30(2)	-13(2)	-1(2)	11(2)
C6	60(2)	23(2)	24(2)	-9(2)	4(2)	0(2)
C7	24(2)	18(2)	26(2)	-1(1)	-1(1)	1(1)
C8	32(2)	24(2)	34(2)	-7(2)	5(1)	-1(2)
C9	42(2)	19(2)	50(2)	-2(2)	6(2)	-6(2)
C10	43(2)	18(2)	51(2)	-4(2)	2(2)	3(2)
C11	48(2)	26(2)	40(2)	-12(2)	4(2)	12(2)
C12	36(2)	26(2)	29(2)	-6(2)	2(2)	4(2)
C13	30(2)	19(2)	25(2)	-4(1)	7(1)	-2(1)
C14	31(2)	20(2)	33(2)	-7(2)	11(1)	3(1)
C15	41(2)	26(2)	44(2)	-1(2)	20(2)	-1(2)
C16	60(3)	40(2)	42(2)	-11(2)	29(2)	-13(2)
C17	58(3)	66(3)	29(2)	-7(2)	9(2)	-12(2)
C18	40(2)	40(2)	27(2)	-1(2)	4(2)	-4(2)
C19	31(2)	19(2)	28(2)	-4(2)	6(1)	-1(2)
C20	34(2)	22(2)	29(2)	-4(2)	8(1)	-1(2)

The complete temperature factor is

$$\exp[-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2$$

$$+ 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl)].$$

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Table 4S. Interatomic distances(Å) involving non-H atoms with e.s.d.'s in parentheses for Cu(I) Polymer.

from	to	distance
Cu	N	2.044(3)
Cu	P	2.197(1)
Cu	Cl'	2.378(1)
Cu	Cl	2.381(1)
P	C1	1.822(3)
P	C7	1.824(3)
P	C13	1.825(3)
N	C19	1.336(4)
N	C20	1.341(4)
C1	C6	1.382(4)
C1	C2	1.388(5)
C2	C3	1.386(5)
C3	C4	1.375(5)
C4	C5	1.377(6)
C5	C6	1.382(5)
C7	C8	1.388(4)
C7	C12	1.389(4)
C8	C9	1.392(5)
C9	C10	1.382(5)
C10	C11	1.380(5)
C11	C12	1.393(5)
C13	C14	1.393(4)
C13	C18	1.393(4)
C14	C15	1.393(5)
C15	C16	1.370(5)
C16	C17	1.375(6)
C17	C18	1.387(5)
C19	C20'	1.382(4)

Table 5S. Bond angles(°) involving non-H atoms with e.s.d.'s in parentheses for Cu(I) Polymer.

from	thru	to	angle
N	Cu	P	120.97(7)
N	Cu	Cl	112.77(7)
N	Cu	Cl	103.49(8)
P	Cu	Cl	107.22(4)
P	Cu	Cl	110.31(4)
Cl	Cu	Cl	100.00(4)
Cu	Cl	Cu	80.00(4)
C1	P	C7	101.8(1)
C1	P	C13	105.6(1)
C1	P	Cu	116.1(1)
C7	P	C13	104.5(1)
C7	P	Cu	113.2(1)
C13	P	Cu	114.3(1)
C19	N	C20	116.2(3)
C19	N	Cu	122.2(2)
C19	N	C19	86.7(2)
C20	N	Cu	121.3(2)
C20	N	C20	86.6(2)
C6	C1	C2	118.7(3)
C6	C1	P	118.5(2)
C2	C1	P	122.8(2)
C2	C1	C5	89.0(2)
C3	C2	C1	120.8(3)
C3	C2	C6	90.2(2)
C1	C2	C4	90.8(2)
C4	C3	C2	119.7(3)
C2	C3	C5	89.7(2)
C3	C4	C5	120.0(3)
C3	C4	C6	90.1(2)
C5	C4	C2	89.7(2)
C4	C5	C6	120.2(3)
C4	C5	C1	90.5(2)
C6	C5	C3	90.3(2)
C1	C6	C5	120.5(3)
C1	C6	C4	90.7(2)
C5	C6	C2	89.8(2)
C8	C7	C12	119.9(3)
C8	C7	P	116.0(2)
C12	C7	P	124.1(2)
C7	C8	C9	119.9(3)
C10	C9	C8	120.2(3)
C8	C9	C11	90.2(2)
C11	C10	C9	119.9(3)
C10	C11	C12	120.4(3)
C12	C11	C9	90.3(2)
C7	C12	C11	119.7(3)
C14	C13	C18	119.2(3)
C14	C13	P	123.9(2)
C18	C13	P	116.9(2)
C13	C14	C15	120.1(3)
C13	C14	C16	90.5(2)
C16	C15	C14	120.2(3)
C14	C15	C17	90.2(2)
C15	C16	C17	120.1(3)
C17	C16	C14	89.9(2)
C16	C17	C18	120.7(3)
C18	C17	C15	90.9(2)
C17	C18	C13	119.7(3)

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N	C19	C20	121.9(3)
N	C19	N	93.3(2)
C20	C19	C20	89.9(2)
N	C20	C19	121.9(3)
N	C20	N	93.4(2)
C19	C20	C19	90.1(2)

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