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P-1090-NCI

X-ray Experimental for $(C_{42}H_{46}N_6)Cu_2Cl_2$-$3CHCl_3$: Crystals grew as very dark, almost black, needles by vapor diffusion of hexanes into a $CHCl_3$ solution of the complex. The data crystal was a needle that tapered to a point at each end and was of approximate dimensions; 0.17x0.17x1.2 mm. The data were collected at 193 K on a Nicolet P3 diffractometer, equipped with a Nicolet LT-2 low-temperature device and using a graphite monochromator with MoKα radiation (λ = 0.71073Å). Details of crystal data, data collection and structure refinement are listed in Supplementary Table 1. Four reflections (1,3,3; 7,1,-2; -1,-3,-3; -6,-2,2) were remeasured every 96 reflections to monitor instrument and crystal stability. A smoothed curve of the intensities of these check reflections was used to scale the data. The scaling factor ranged from 0.990 to 1.01. The data were corrected for Lp effects but not absorption. Data reduction and decay correction were performed using the SHELXTL-*Plus* software package.[1] The structure was solved by direct methods and refined on F^2 by full-matrix least-squares[2] with anisotropic thermal parameters for the non-H atoms. All hydrogen atoms were calculated in idealized positions (C-H 0.96Å) with Uiso set to 0.08. There are three molecules of $CHCl_3$ solvate in the lattice. One molecule was found to be disordered by rotation of the chlorine atoms. Six Cl positions were refined. The major component of the disorder had a site occupancy factor that refined to 77(1)%. These atoms Cl1a, Cl2a and Cl3a were refined anisotropically. The atoms of the minor component, Cl1', Cl2' and Cl3' were refined isotropically. The carbon atom of the third $CHCl_3$ molecule, C1c, was also refined isotropically. The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.02*P)^2]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[3] Other computer programs used in this work are listed elsewhere.[4] All figures were generated using SHELXTL-*Plus*.[1] Tables of positional and thermal parameters, bond lengths, angles and torsion angles, and additional figures now follow.

References

1) Sheldrick, G. M. SHELXTL-*PLUS* (Version 4.1). Siemens Analytical X-ray Instruments, Inc.: Madison, Wisconsin, USA **1990.**

2) Sheldrick, G. M. SHELXL (1994). A program to refine crystal structures from X-ray and neutron diffraction data. *J. Appl. Cryst.* in preparation.

3) International Tables for X-ray Crystallography (1992). Vol. C, Tables 4.2.6.8 and 6.1.1.4, Wilson, A. J. C., Ed., Kluwer Academic Press: Boston, USA **1992.**

4) Gadol, S. M.; Davis, R. E. *Organometallics* **1982,***1*, 1607-1613.

R-1090-M3

Supplementary Table 1. Crystallographic Data[a] for $(C_{42}H_{46}N_6)Cu_2Cl_2$-$3CHCl_3$.

Formula	$C_{45}H_{49}N_6Cl_{11}Cu_2$
fw	1190.93
a, Å	23.889(8)
b, Å	13.602(4)
c, Å	32.350(9)
β, °	100.41(2)
V, $Å^3$	10339(5)
Z	8
F(000)	4680
Crystal System	Monoclinic
Space Group	C2/C
T, °C	-80
2θ range (°)	4 - 50
Scan speed (°/min) (1.2° ω scan)	4 - 8
ρcalc, g/cc	1.53
Reflections measured	9353
Unique reflections	9119
Decay Correction	0.990 - 1.01
R_{int} (F^2)	0.054

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Supplementary Table 1. (continued).

μ, cm-1	15.3
Crystal size, mm	0.17x0.17x1.2
Transmission factor range	N/A
$R_w(F^2)$[b]	0.152
R(F)[c]	0.0827
Goodness of fit, $S(F^2)$[d]	1.795
Parameters	578
Max $\lvert\Delta/\sigma\rvert$	<0.1
Min, max peaks ($e^-/Å^3$)	-0.67, 1.13

[a] Data were collected on a Nicolet P3 diffractometer using graphite monochromatized Mo Kα radiation (λ = 0.71073Å). Lattice parameters were obtained from the least-squares refinement of 40 reflections with $16.2 < 2\theta < 23.7°$.

[b] $R_w = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|^4\}^{1/2}$ and where the weight, w, is defined as follows:

$w = 1/\{\sigma^2(|F_o|^2) + (0.02P)^2\}$; P = [1/3*(Maximum of (0 or $|F_o|^2$) + 2/3*$|F_c|^2$].

[c] The conventional R index based on F where 5116 reflections have $F_o > 4(\sigma(F_o))$.

[d] $S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

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Supplementary Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($Å^2$) for the non-hydrogen atoms of $(C_{42}H_{46}N_6)Cu_2Cl_2$-$3CHCl_3$.

Atom	x	y	z	U
Cu1	0.09372(4)	0.55034(7)	0.33751(3)	0.0305(4)
Cu2	0.12417(4)	0.63291(7)	0.41635(3)	0.0317(4)
Cl1	0.19198(8)	0.5533(2)	0.37823(6)	0.0333(7)
Cl2	0.03039(8)	0.62819(14)	0.37555(5)	0.0305(7)
N1	0.1014(3)	0.6682(4)	0.3022(2)	0.025(2)
N2	0.1450(3)	0.7599(4)	0.3904(2)	0.030(2)
N3	0.1527(3)	0.7071(5)	0.4659(2)	0.033(3)
N4	0.1077(3)	0.5193(5)	0.4518(2)	0.031(2)
N5	0.0882(3)	0.4168(4)	0.3642(2)	0.029(2)
N6	0.0809(3)	0.4689(4)	0.2879(2)	0.031(3)
C1	0.0780(3)	0.6692(6)	0.2598(2)	0.029(3)
C2	0.0731(3)	0.7692(6)	0.2449(2)	0.030(3)
C3	0.0956(3)	0.8275(6)	0.2772(2)	0.029(3)
C4	0.1150(3)	0.7630(6)	0.3125(2)	0.027(3)
C5	0.1461(3)	0.7960(5)	0.3516(2)	0.027(3)
C6	0.1848(3)	0.8800(6)	0.3564(2)	0.030(3)
C7	0.2035(3)	0.8967(6)	0.3982(2)	0.031(3)
C8	0.1775(3)	0.8201(5)	0.4195(2)	0.027(3)
C9	0.1781(3)	0.7958(6)	0.4620(2)	0.032(3)
C10	0.1929(3)	0.8417(6)	0.5026(2)	0.034(3)
C11	0.1753(3)	0.7791(6)	0.5304(2)	0.036(3)
C12	0.1495(3)	0.6935(6)	0.5068(2)	0.032(3)
C13	0.1231(3)	0.6097(6)	0.5183(2)	0.032(3)
C14	0.1026(3)	0.5321(6)	0.4928(2)	0.030(3)
C15	0.0732(3)	0.4505(6)	0.5071(2)	0.033(3)
C16	0.0627(3)	0.3853(6)	0.4746(2)	0.034(3)
C17	0.0868(3)	0.4277(6)	0.4402(2)	0.033(3)
C18	0.0912(3)	0.3765(6)	0.4023(2)	0.032(3)
C19	0.1000(3)	0.2710(6)	0.3992(3)	0.038(3)
C20	0.0990(4)	0.2503(6)	0.3581(3)	0.038(3)
C21	0.0904(3)	0.3407(5)	0.3361(3)	0.033(3)
C22	0.0841(3)	0.3695(6)	0.2938(2)	0.032(3)
C23	0.0751(4)	0.3246(6)	0.2521(3)	0.038(3)
C24	0.0657(3)	0.3990(6)	0.2230(2)	0.031(3)
C25	0.0708(3)	0.4909(6)	0.2469(2)	0.031(3)
C26	0.0654(3)	0.5871(6)	0.2334(2)	0.031(3)
C27	0.0495(4)	0.7997(6)	0.2009(2)	0.041(3)
C28	0.0964(4)	0.8043(7)	0.1742(3)	0.068(4)
C29	0.0911(3)	0.9375(5)	0.2776(2)	0.042(3)
C30	0.2129(3)	0.9266(6)	0.3220(2)	0.045(4)
C31	0.2446(3)	0.9738(6)	0.4170(2)	0.045(3)
C32	0.2192(4)	0.9394(6)	0.5131(2)	0.049(4)
C33	0.1777(4)	0.7918(7)	0.5771(2)	0.046(4)
C34	0.1225(4)	0.8349(7)	0.5859(3)	0.070(5)
C35	0.0565(3)	0.4386(6)	0.5497(2)	0.040(3)
C36	0.1016(4)	0.3868(7)	0.5805(3)	0.058(4)

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Supplementary Table 2. (continued).

Atom	x	y	z	U
C37	0.0260(4)	0.2954(6)	0.4728(3)	0.050(4)
C38	0.1174(4)	0.1990(6)	0.4350(3)	0.057(4)
C39	0.1094(4)	0.1507(6)	0.3407(3)	0.067(5)
C40	0.0757(4)	0.2167(6)	0.2419(3)	0.055(4)
C41	0.0560(3)	0.3937(6)	0.1762(2)	0.037(3)
C42	0.1119(4)	0.3972(7)	0.1597(3)	0.063(4)
C1B	0.2623(5)	0.3367(7)	0.4019(3)	0.078(5)
Cl1B	0.2554(2)	0.2432(3)	0.36426(11)	0.113(2)
Cl2B	0.3277(2)	0.3952(3)	0.40269(13)	0.131(2)
Cl3B	0.2620(2)	0.2861(3)	0.45103(11)	0.135(2)
C1A	0.2391(6)	0.5820(9)	0.2845(3)	0.089(6)
Cl1A	0.2221(2)	0.4548(4)	0.26945(14)	0.110(2)
Cl2A	0.2244(3)	0.6619(6)	0.2416(3)	0.180(4)
Cl3A	0.3106(2)	0.5784(4)	0.30650(13)	0.119(2)
Cl1'	0.2611(14)	0.484(3)	0.2842(9)	0.231(14)
Cl2'	0.2160(9)	0.6118(11)	0.2367(6)	0.069(5)
Cl3'	0.2803(10)	0.687(2)	0.3038(7)	0.186(9)
C1C	-0.0285(3)	0.1157(4)	0.5703(2)	0.054(5)
Cl1C	-0.0308(3)	0.0361(5)	0.61326(13)	0.140(4)
Cl2C	0.0431(3)	0.1245(7)	0.5652(2)	0.156(5)
Cl3C	-0.0635(2)	0.0565(6)	0.52564(14)	0.141(4)

For anisotropic atoms, the U value is U_{eq}, calculated as $U_{eq} = 1/3\ \Sigma_i\Sigma_j\ U_{ij}\ a_i^*\ a_j^*\ A_{ij}$ where A_{ij} is the dot product of the i^{th} and j^{th} direct space unit cell vectors.

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Supplementary Table 3. Anisotropic thermal parameters for the non-hydrogen atoms of $(C_{42}H_{46}N_6)Cu_2Cl_2$-$3CHCl_3$.

Atom	U11	U22	U33	U12	U13	U23
Cu1	0.0463(7)	0.0229(6)	0.0250(5)	-0.0035(6)	0.0136(5)	-0.0032(5)
Cu2	0.0478(7)	0.0264(6)	0.0230(5)	-0.0075(6)	0.0121(5)	-0.0022(5)
Cl1	0.0353(13)	0.0362(12)	0.0307(11)	0.0001(11)	0.0122(10)	-0.0035(10)
Cl2	0.0329(13)	0.0340(12)	0.0276(10)	0.0028(11)	0.0134(9)	0.0030(10)
N1	0.031(4)	0.023(4)	0.025(4)	0.002(3)	0.016(3)	-0.001(3)
N2	0.044(5)	0.023(4)	0.024(4)	-0.002(3)	0.013(3)	0.001(3)
N3	0.053(5)	0.029(4)	0.019(4)	0.001(4)	0.009(3)	-0.002(3)
N4	0.043(5)	0.027(4)	0.026(4)	-0.006(3)	0.016(3)	-0.003(3)
N5	0.041(4)	0.023(4)	0.026(4)	-0.001(3)	0.011(3)	0.004(3)
N6	0.044(5)	0.027(4)	0.026(4)	-0.006(3)	0.012(3)	-0.004(3)
C1	0.027(5)	0.033(5)	0.027(5)	0.004(4)	0.010(4)	-0.002(4)
C2	0.033(5)	0.041(5)	0.017(4)	0.007(4)	0.010(4)	0.004(4)
C3	0.037(5)	0.026(5)	0.027(4)	-0.002(4)	0.018(4)	-0.003(4)
C4	0.032(5)	0.027(5)	0.026(4)	-0.004(4)	0.018(4)	-0.002(4)
C5	0.032(5)	0.021(4)	0.033(5)	-0.007(4)	0.015(4)	-0.004(4)
C6	0.027(5)	0.032(5)	0.030(5)	0.001(4)	0.004(4)	0.002(4)
C7	0.029(5)	0.030(5)	0.033(5)	-0.007(4)	0.002(4)	-0.005(4)
C8	0.033(5)	0.023(5)	0.026(4)	0.001(4)	0.004(4)	-0.003(4)
C9	0.041(6)	0.030(5)	0.027(5)	0.002(4)	0.010(4)	-0.004(4)
C10	0.035(5)	0.043(6)	0.023(4)	-0.005(4)	0.001(4)	-0.010(4)
C11	0.035(6)	0.044(6)	0.030(5)	0.003(5)	0.010(4)	-0.004(4)
C12	0.035(5)	0.038(5)	0.025(5)	0.004(5)	0.010(4)	-0.006(4)
C13	0.033(5)	0.039(6)	0.026(4)	0.008(4)	0.013(4)	0.003(4)
C14	0.036(5)	0.030(5)	0.026(4)	0.001(4)	0.010(4)	0.003(4)
C15	0.034(5)	0.037(5)	0.030(4)	-0.008(5)	0.013(4)	0.004(4)
C16	0.034(5)	0.026(5)	0.041(5)	-0.004(4)	0.003(4)	0.011(4)
C17	0.042(6)	0.025(5)	0.034(5)	0.003(4)	0.016(4)	0.011(4)
C18	0.029(5)	0.027(5)	0.037(5)	-0.005(4)	0.002(4)	0.003(4)
C19	0.044(6)	0.023(5)	0.046(6)	-0.003(4)	0.009(5)	0.008(4)
C20	0.049(6)	0.023(5)	0.045(5)	-0.001(4)	0.014(5)	-0.002(4)
C21	0.048(6)	0.019(5)	0.035(5)	0.011(4)	0.018(4)	-0.000(4)
C22	0.035(5)	0.023(5)	0.039(5)	0.003(4)	0.011(4)	-0.008(4)
C23	0.049(6)	0.026(5)	0.041(5)	-0.002(4)	0.011(5)	-0.018(4)
C24	0.034(5)	0.029(5)	0.035(5)	-0.005(4)	0.017(4)	-0.013(4)
C25	0.035(6)	0.035(5)	0.026(5)	-0.001(4)	0.012(4)	-0.005(4)
C26	0.037(6)	0.037(5)	0.021(4)	0.001(4)	0.012(4)	-0.008(4)
C27	0.061(7)	0.033(5)	0.028(5)	-0.004(5)	0.007(4)	-0.006(4)
C28	0.093(9)	0.087(8)	0.034(5)	-0.019(7)	0.036(6)	-0.006(5)
C29	0.050(6)	0.031(5)	0.044(5)	-0.006(5)	0.009(5)	-0.006(4)
C30	0.046(6)	0.047(6)	0.049(5)	-0.014(5)	0.024(5)	0.001(5)
C31	0.046(6)	0.048(6)	0.043(5)	-0.014(5)	0.008(5)	-0.005(4)
C32	0.061(7)	0.048(6)	0.042(5)	-0.011(5)	0.019(5)	-0.016(5)
C33	0.058(7)	0.054(6)	0.028(5)	-0.007(5)	0.014(5)	-0.014(5)
C34	0.085(9)	0.081(8)	0.050(6)	-0.010(7)	0.028(6)	-0.028(6)
C35	0.042(6)	0.044(6)	0.037(5)	0.002(5)	0.018(4)	0.010(4)

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Supplementary Table 3. (continued).

Atom	U11	U22	U33	U12	U13	U23
C36	0.065(7)	0.070(7)	0.040(6)	0.004(6)	0.008(5)	0.022(5)
C37	0.051(6)	0.043(6)	0.062(6)	-0.003(5)	0.026(5)	0.010(5)
C38	0.083(8)	0.036(6)	0.057(6)	0.011(6)	0.024(6)	0.013(5)
C39	0.107(9)	0.029(6)	0.073(7)	0.002(6)	0.033(7)	-0.010(5)
C40	0.085(8)	0.037(6)	0.047(6)	-0.006(6)	0.019(5)	-0.013(5)
C41	0.042(6)	0.037(5)	0.036(5)	-0.000(4)	0.016(4)	-0.017(4)
C42	0.079(8)	0.084(8)	0.032(5)	0.014(6)	0.021(5)	-0.004(5)
C1B	0.097(10)	0.051(7)	0.097(9)	-0.003(7)	0.046(7)	0.000(6)
Cl1B	0.115(3)	0.108(3)	0.117(3)	0.023(2)	0.023(2)	-0.013(2)
Cl2B	0.157(4)	0.086(3)	0.186(4)	-0.015(2)	0.123(3)	-0.033(3)
Cl3B	0.158(4)	0.156(4)	0.102(3)	-0.029(3)	0.055(3)	0.021(3)
C1A	0.108(11)	0.097(10)	0.075(8)	0.017(9)	0.049(8)	0.011(7)
Cl1A	0.077(3)	0.169(5)	0.100(3)	-0.033(3)	0.053(3)	-0.064(3)
Cl2A	0.171(7)	0.188(8)	0.219(7)	0.087(6)	0.132(6)	0.131(7)
Cl3A	0.073(3)	0.197(6)	0.081(3)	-0.047(4)	-0.002(2)	0.029(3)
Cl1C	0.201(8)	0.153(7)	0.078(4)	-0.128(6)	0.059(5)	-0.032(5)
Cl2C	0.191(9)	0.197(9)	0.084(5)	-0.075(8)	0.034(5)	0.013(6)
Cl3C	0.112(6)	0.215(9)	0.099(5)	0.042(6)	0.024(5)	0.030(6)

The Uij are the mean-square amplitudes of vibration in $Å^2$ from the general temperature factor expression

$$\exp[-2\pi^2(h^2a^{*2}U11 + k^2b^{*2}U22 + l^2c^{*2}U33 + 2hka^*b^*U12 + 2hla^*c^*U13 + 2klb^*c^*U23)]$$

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Supplementary Table 4. Fractional coordinates and isotropic thermal parameters ($Å^2$) for the hydrogen atoms of $(C_{42}H_{46}N_6)Cu_2Cl_2$-$3CHCl_3$.

Atom	x	y	z	U
H13	0.1193	0.6055	0.5473	0.08
H26	0.0512	0.5983	0.2042	0.08
H27A	0.0313	0.8626	0.2009	0.08
H27B	0.0218	0.7524	0.1882	0.08
H28A	0.0821	0.8236	0.1458	0.08
H28B	0.1237	0.8518	0.1872	0.08
H28C	0.1142	0.7410	0.1745	0.08
H29A	0.0765	0.9609	0.2498	0.08
H29B	0.0659	0.9568	0.2962	0.08
H29C	0.1280	0.9652	0.2872	0.08
H30A	0.2371	0.9799	0.3334	0.08
H30B	0.2348	0.8779	0.3105	0.08
H30C	0.1835	0.9510	0.3002	0.08
H31A	0.2549	1.0143	0.3952	0.08
H31B	0.2275	1.0139	0.4357	0.08
H31C	0.2780	0.9426	0.4323	0.08
H32A	0.2244	0.9495	0.5429	0.08
H32B	0.2553	0.9427	0.5042	0.08
H32C	0.1946	0.9896	0.4991	0.08
H33A	0.2085	0.8344	0.5888	0.08
H33B	0.1836	0.7289	0.5907	0.08
H34A	0.1227	0.8430	0.6154	0.08
H34B	0.1171	0.8978	0.5722	0.08
H34C	0.0921	0.7916	0.5741	0.08
H35A	0.0219	0.4015	0.5465	0.08
H35B	0.0500	0.5021	0.5609	0.08
H36A	0.0910	0.3785	0.6075	0.08
H36B	0.1076	0.3234	0.5689	0.08
H36C	0.1359	0.4246	0.5834	0.08
H37A	0.0157	0.2829	0.4996	0.08
H37B	-0.0077	0.3072	0.4523	0.08
H37C	0.0458	0.2394	0.4644	0.08
H38A	0.1201	0.1343	0.4237	0.08
H38B	0.1534	0.2176	0.4512	0.08
H38C	0.0891	0.1992	0.4527	0.08
H39A	0.1145	0.1032	0.3630	0.08
H39B	0.0774	0.1326	0.3198	0.08
H39C	0.1429	0.1528	0.3282	0.08
H40A	0.0686	0.2087	0.2119	0.08
H40B	0.1120	0.1889	0.2534	0.08
H40C	0.0465	0.1837	0.2535	0.08
H41A	0.0321	0.4473	0.1645	0.08
H41B	0.0369	0.3331	0.1672	0.08
H42A	0.1054	0.3933	0.1296	0.08
H42B	0.1306	0.4581	0.1686	0.08
H42C	0.1354	0.3432	0.1713	0.08

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Supplementary Table 5. Bond Lengths (Å) and Angles (°) for the non-hydrogen atoms of $(C_{42}H_{46}N_6)Cu_2Cl_2-3CHCl_3$.

1	2	3	1-2	1-2-3
Cu2	Cu1	Cl1	2.7613(15)	55.65(6)
Cu2	Cu1	Cl2		54.83(5)
Cu2	Cu1	N1		99.6(2)
Cu2	Cu1	N5		89.9(2)
Cu2	Cu1	N6		168.0(2)
Cl1	Cu1	Cl2	2.476(2)	110.48(7)
Cl1	Cu1	N1		96.6(2)
Cl1	Cu1	N5		85.2(2)
Cl1	Cu1	N6		116.4(2)
Cl2	Cu1	N1	2.366(2)	94.1(2)
Cl2	Cu1	N5		94.7(2)
N6	Cu1	Cl2	1.928(6)	132.0(2)
N1	Cu1	N5	1.997(6)	169.7(2)
N1	Cu1	N6		90.1(2)
N5	Cu1	N6	2.026(6)	80.0(2)
Cl1	Cu2	Cl2	2.458(2)	110.40(7)
Cl1	Cu2	N2		86.2(2)
Cl1	Cu2	N3		119.1(2)
Cl1	Cu2	N4		99.4(2)
Cl1	Cu2	Cu1		56.28(5)
Cl2	Cu2	N2	2.387(2)	94.0(2)
Cl2	Cu2	N3		129.4(2)
Cl2	Cu2	N4		92.0(2)
Cl2	Cu2	Cu1		54.13(5)
N2	Cu2	N3	2.021(6)	79.6(2)
N2	Cu2	N4		169.8(2)
N2	Cu2	Cu1		90.5(2)
N3	Cu2	N4	1.912(6)	90.2(2)
N3	Cu2	Cu1		169.5(2)
N4	Cu2	C8	2.006(6)	143.5(2)
N4	Cu2	C9		114.9(2)
N4	Cu2	Cu1		99.7(2)
Cu1	Cl1	Cu2		68.07(6)
Cu1	Cl2	Cu2		71.04(7)
C1	N1	C4	1.383(9)	105.7(6)
C1	N1	Cu1		120.8(5)
C4	N1	Cu1	1.356(10)	131.7(5)
C5	N2	C8	1.354(10)	108.3(6)
C5	N2	Cu2		138.0(5)
C8	N2	Cu2	1.375(9)	112.1(5)
C9	N3	C12	1.366(10)	108.4(6)
C9	N3	Cu2		119.0(5)
C12	N3	Cu2	1.350(10)	132.3(5)
C14	N4	C17	1.365(10)	106.9(6)
C14	N4	Cu2		121.3(5)
C17	N4	Cu2	1.370(10)	130.0(5)
C18	N5	C21	1.339(10)	107.3(6)

Supplementary Table 5. (continued).

1	2	3	1-2	1-2-3
C18	N5	Cu1		139.7(5)
C21	N5	Cu1	1.385(10)	112.1(5)
C22	N6	C25	1.365(10)	110.7(6)
C22	N6	Cu1		117.2(5)
C25	N6	Cu1	1.340(10)	132.1(5)
C2	C1	C26	1.443(11)	123.4(7)
C2	C1	N1		109.6(6)
C26	C1	N1	1.404(11)	126.8(7)
C3	C2	C27	1.345(10)	127.5(7)
C3	C2	C1		107.3(6)
C27	C2	C1	1.491(10)	125.2(7)
C4	C3	C29	1.447(10)	127.7(7)
C4	C3	C2		106.4(7)
C29	C3	C2	1.501(11)	125.0(7)
C5	C4	N1	1.419(10)	125.7(7)
C5	C4	C3		123.5(7)
N1	C4	C3		110.7(6)
C6	C5	N2	1.461(11)	107.7(6)
C6	C5	C4		124.1(7)
N2	C5	C4		128.2(7)
C7	C6	C30	1.367(10)	122.8(7)
C7	C6	C5		108.8(7)
C30	C6	C5	1.534(12)	126.7(6)
C8	C7	C31	1.449(11)	128.5(7)
C8	C7	C6		105.0(6)
C31	C7	C6	1.489(11)	126.4(7)
C9	C8	Cu2	1.413(10)	75.5(4)
C9	C8	N2		115.5(7)
C9	C8	C7		134.4(7)
Cu2	C8	N2		41.2(3)
Cu2	C8	C7		148.9(5)
N2	C8	C7		110.0(6)
C10	C9	Cu2	1.439(10)	145.8(6)
C10	C9	N3		109.8(7)
C10	C9	C8		138.1(7)
Cu2	C9	N3		36.1(3)
Cu2	C9	C8		75.7(4)
N3	C9	C8		111.7(6)
C11	C10	C32	1.359(12)	125.3(7)
C11	C10	C9		106.1(7)
C32	C10	C9	1.484(11)	128.5(7)
C12	C11	C33	1.466(11)	123.2(7)
C12	C11	C10		107.6(7)
C33	C11	C10	1.512(11)	129.1(7)
C13	C12	N3	1.386(12)	119.0(7)
C13	C12	C11		132.9(7)
N3	C12	C11		108.0(7)
C14	C13	C12	1.374(10)	126.9(7)
C15	C14	N4	1.433(11)	110.4(6)

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Supplementary Table 5. (continued).

1	2	3	1-2	1-2-3
C15	C14	C13		123.0(7)
N4	C14	C13		126.6(7)
C16	C15	C35	1.363(11)	126.2(7)
C16	C15	C14		106.8(7)
C35	C15	C14	1.511(11)	127.0(7)
C17	C16	C37	1.461(12)	126.8(7)
C17	C16	C15		106.7(7)
C37	C16	C15	1.498(11)	126.0(8)
C18	C17	N4	1.430(11)	126.8(7)
C18	C17	C16		124.1(7)
N4	C17	C16		108.9(7)
C19	C18	N5	1.456(11)	109.0(7)
C19	C18	C17		124.9(7)
N5	C18	C17		126.1(7)
C20	C19	C38	1.357(12)	124.7(7)
C20	C19	C18		107.1(7)
C38	C19	C18	1.515(11)	127.4(7)
C21	C20	C39	1.417(11)	127.8(8)
C21	C20	C19		106.8(7)
C39	C20	C19	1.505(12)	125.3(7)
C22	C21	Cu1	1.405(11)	74.6(4)
C22	C21	N5		114.9(6)
C22	C21	C20		135.4(7)
Cu1	C21	N5		41.2(3)
Cu1	C21	C20		149.1(6)
N5	C21	C20		109.7(7)
C23	C22	Cu1	1.461(11)	144.3(5)
C23	C22	N6		107.0(6)
C23	C22	C21		139.0(7)
Cu1	C22	N6		37.3(3)
Cu1	C22	C21		76.7(4)
N6	C22	C21		113.9(7)
C24	C23	C40	1.373(11)	125.2(7)
C24	C23	C22		107.6(7)
C40	C23	C22	1.505(11)	127.2(7)
C25	C24	C41	1.463(11)	124.1(7)
C25	C24	C23		106.3(7)
C41	C24	C23	1.491(10)	129.5(7)
C26	C25	N6	1.377(11)	120.9(7)
C26	C25	C24		130.6(7)
N6	C25	C24		108.4(7)
C1	C26	C25		124.5(7)
C28	C27	C2	1.533(13)	111.1(7)
C34	C33	C11	1.516(14)	110.7(6)
C36	C35	C15	1.504(11)	112.3(7)
C42	C41	C24	1.527(13)	111.6(6)
Cl1B	C1B	Cl2B	1.748(11)	108.2(7)
Cl2B	C1B	Cl3B	1.749(12)	108.6(6)
Cl3B	C1B	Cl1B	1.734(12)	109.5(6)

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Supplementary Table 5. (continued).

1	2	3	1-2	1-2-3
Cl2A	C1A	Cl3A	1.747(14)	112.8(8)
Cl2A	C1A	Cl1'		126.6(15)
Cl2A	C1A	Cl2'		24.4(6)
Cl3A	C1A	Cl1'	1.728(13)	69.0(14)
Cl3A	C1A	Cl2'		123.4(11)
Cl3A	C1A	Cl3'		55.6(9)
Cl1'	C1A	Cl2'	1.44(4)	107.1(15)
Cl1'	C1A	Cl3'		125.(2)
Cl2'	C1A	Cl3'	1.60(2)	102.1(12)
Cl3'	C1A	Cl2A	1.78(3)	78.5(9)
Cl1C	C1C	Cl2C	1.770(8)	106.6(4)
Cl2C	C1C	Cl3C	1.752(9)	106.6(4)
Cl3C	C1C	Cl1C	1.733(7)	106.9(4)

P-1090-M14

Supplementary Table 6. Bond Lengths (Å) and Angles (°) for the hydrogen atoms of $(C_{42}H_{46}N_6)Cu_2Cl_2$-$3CHCl_3$.

1	2	3	1-2	1-2-3
H13	C13	C14	0.96	117.0(9)
H13	C13	C12		116.1(9)
H26	C26	C1	0.96	118.2(9)
H26	C26	C25		117.3(9)
H27A	C27	H27B	0.96	108.7(10)
H27A	C27	C28		109.9(9)
H27A	C27	C2		109.9(8)
H27B	C27	C28	0.96	107.7(9)
H27B	C27	C2		109.5(8)
H28A	C28	H28B	0.96	109.4(12)
H28A	C28	H28C		109.4(12)
H28A	C28	C27		112.5(10)
H28B	C28	H28C	0.96	109.6(12)
H28B	C28	C27		106.8(10)
H28C	C28	C27	0.96	109.0(10)
H29A	C29	H29B	0.96	109.6(10)
H29A	C29	H29C		109.3(10)
H29A	C29	C3		109.8(8)
H29B	C29	H29C	0.96	109.4(10)
H29B	C29	C3		109.4(8)
H29C	C29	C3	0.96	109.3(8)
H30A	C30	H30B	0.96	109.6(11)
H30A	C30	H30C		109.3(10)
H30A	C30	C6		110.2(9)
H30B	C30	H30C	0.96	109.4(10)
H30B	C30	C6		109.7(9)
H30C	C30	C6	0.96	108.5(9)
H31A	C31	H31B	0.96	109.4(10)
H31A	C31	H31C		109.5(11)
H31A	C31	C7		110.1(8)
H31B	C31	H31C	0.96	109.5(10)
H31B	C31	C7		109.4(9)
H31C	C31	C7	0.96	108.9(9)
H32A	C32	H32B	0.96	109.6(10)
H32A	C32	H32C		109.4(11)
H32A	C32	C10		109.3(9)
H32B	C32	H32C	0.96	109.4(11)
H32B	C32	C10		109.8(9)
H32C	C32	C10	0.96	109.3(8)
H33A	C33	H33B	0.96	108.7(10)
H33A	C33	C34		108.8(10)
H33A	C33	C11		110.5(9)
H33B	C33	C34	0.96	108.7(10)
H33B	C33	C11		109.4(9)
H34A	C34	H34B	0.96	109.4(12)
H34A	C34	H34C		109.4(13)
H34A	C34	C33		112.5(10)

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Supplementary Table 6. (continued).

1	2	3	1-2	1-2-3
H34B	C34	H34C	0.96	109.6(11)
H34B	C34	C33		107.8(11)
H34C	C34	C33	0.96	108.0(10)
H35A	C35	H35B	0.96	108.6(11)
H35A	C35	C36		109.0(9)
H35A	C35	C15		108.9(8)
H35B	C35	C36	0.96	108.4(8)
H35B	C35	C15		109.6(9)
H36A	C36	H36B	0.96	109.5(12)
H36A	C36	H36C		109.5(10)
H36A	C36	C35		112.6(10)
H36B	C36	H36C	0.96	109.5(12)
H36B	C36	C35		107.6(8)
H36C	C36	C35	0.96	108.1(9)
H37A	C37	H37B	0.96	109.5(11)
H37A	C37	H37C		109.5(11)
H37A	C37	C16		110.6(9)
H37B	C37	H37C	0.96	109.4(10)
H37B	C37	C16		107.6(9)
H37C	C37	C16	0.96	110.2(9)
H38A	C38	H38B	0.96	109.5(12)
H38A	C38	H38C		109.5(12)
H38A	C38	C19		109.2(9)
H38B	C38	H38C	0.96	109.4(11)
H38B	C38	C19		110.0(9)
H38C	C38	C19	0.96	109.2(9)
H39A	C39	H39B	0.96	109.4(12)
H39A	C39	H39C		109.5(12)
H39A	C39	C20		109.5(10)
H39B	C39	H39C	0.96	109.4(12)
H39B	C39	C20		109.3(10)
H39C	C39	C20	0.96	109.8(9)
H40A	C40	H40B	0.96	109.4(12)
H40A	C40	H40C		109.6(11)
H40A	C40	C23		108.9(8)
H40B	C40	H40C	0.96	109.4(11)
H40B	C40	C23		110.0(9)
H40C	C40	C23	0.96	109.5(10)
H41A	C41	H41B	0.96	108.5(9)
H41A	C41	C42		109.5(9)
H41A	C41	C24		109.6(8)
H41B	C41	C42	0.96	108.7(9)
H41B	C41	C24		109.0(8)
H42A	C42	H42B	0.96	109.4(12)
H42A	C42	H42C		109.4(12)
H42A	C42	C41		111.1(9)
H42B	C42	H42C	0.96	109.6(11)
H42B	C42	C41		108.2(10)
H42C	C42	C41	0.96	109.1(10)

P-1090-M14

Supplementary Table 7. Torsion Angles (°) for the non-hydrogen atoms of $(C_{42}H_{46}N_6)Cu_2Cl_2$-$3CHCl_3$.

1	2	3	4	1-2-3-4
C1	N1	C4	C3	5.1(9)
C1	N1	C4	C5	-172.4(8)
C4	N1	C1	C2	-4.8(9)
C4	N1	C1	C26	169.5(8)
C5	N2	C8	C7	-3.1(9)
C5	N2	C8	C9	176.4(7)
C8	N2	C5	C4	-174.3(8)
C8	N2	C5	C6	4.2(8)
C9	N3	C12	C11	-0.8(9)
C9	N3	C12	C13	177.4(7)
C12	N3	C9	C8	-173.7(7)
C12	N3	C9	C10	0.9(9)
C14	N4	C17	C16	5.4(8)
C14	N4	C17	C18	-169.8(7)
C17	N4	C14	C13	173.6(8)
C17	N4	C14	C15	-5.1(8)
C18	N5	C21	C20	-4.0(9)
C18	N5	C21	C22	176.1(7)
C21	N5	C18	C17	-175.9(8)
C21	N5	C18	C19	4.4(9)
C22	N6	C25	C24	1.1(9)
C22	N6	C25	C26	179.5(8)
C25	N6	C22	C21	-175.6(7)
C25	N6	C22	C23	0.1(8)
C2	C1	C26	C25	178.7(8)
C26	C1	C2	C3	-171.8(8)
C26	C1	C2	C27	5.8(13)
N1	C1	C2	C3	2.7(9)
N1	C1	C2	C27	-179.7(9)
N1	C1	C26	C25	5.1(14)
C3	C2	C27	C28	87.3(11)
C27	C2	C3	C4	-177.1(8)
C27	C2	C3	C29	12.7(14)
C1	C2	C3	C4	0.4(10)
C1	C2	C3	C29	-169.7(8)
C1	C2	C27	C28	-89.8(10)
C29	C3	C4	N1	166.3(8)
C29	C3	C4	C5	-16.1(13)
C2	C3	C4	N1	-3.5(10)
C2	C3	C4	C5	174.1(8)
N1	C4	C5	N2	-35.2(13)
N1	C4	C5	C6	146.6(8)
C3	C4	C5	N2	147.6(8)
C3	C4	C5	C6	-30.7(12)
N2	C5	C6	C7	-3.9(9)
N2	C5	C6	C30	161.6(7)
C4	C5	C6	C7	174.7(7)

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Supplementary Table 7. (continued).

1	2	3	4	1-2-3-4
C4	C5	C6	C30	-19.8(12)
C30	C6	C7	C8	-164.2(7)
C30	C6	C7	C31	12.4(13)
C5	C6	C7	C8	1.9(9)
C5	C6	C7	C31	178.6(7)
C31	C7	C8	N2	-175.9(8)
C31	C7	C8	C9	5.(2)
C6	C7	C8	N2	0.7(9)
C6	C7	C8	C9	-178.7(9)
N2	C8	C9	N3	9.4(10)
N2	C8	C9	C10	-163.0(9)
C7	C8	C9	N3	-171.3(8)
C7	C8	C9	C10	16.(2)
N3	C9	C10	C11	-0.6(9)
N3	C9	C10	C32	-177.7(8)
C8	C9	C10	C11	171.8(10)
C8	C9	C10	C32	-5.(2)
C32	C10	C11	C12	177.3(8)
C32	C10	C11	C33	0.1(8)
C9	C10	C11	C12	0.0(8)
C9	C10	C11	C33	-177.1(8)
C12	C11	C33	C34	-83.6(10)
C33	C11	C12	N3	177.9(7)
C33	C11	C12	C13	0.0(8)
C10	C11	C12	N3	0.4(9)
C10	C11	C12	C13	-177.4(9)
C10	C11	C33	C34	93.3(10)
N3	C12	C13	C14	5.4(13)
C11	C12	C13	C14	-177.0(8)
C12	C13	C14	N4	4.7(13)
C12	C13	C14	C15	-176.8(8)
N4	C14	C15	C16	2.7(9)
N4	C14	C15	C35	-176.9(7)
C13	C14	C15	C16	-176.1(7)
C13	C14	C15	C35	4.4(12)
C16	C15	C35	C36	89.4(9)
C35	C15	C16	C17	-180.(45)
C35	C15	C16	C37	8.4(13)
C14	C15	C16	C17	0.7(8)
C14	C15	C16	C37	-171.1(7)
C14	C15	C35	C36	-91.1(10)
C37	C16	C17	N4	167.9(7)
C37	C16	C17	C18	-16.7(12)
C15	C16	C17	N4	-3.9(9)
C15	C16	C17	C18	171.5(7)
N4	C17	C18	N5	-37.1(12)
N4	C17	C18	C19	142.6(8)
C16	C17	C18	N5	148.3(8)
C16	C17	C18	C19	-31.9(12)

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Supplementary Table 7. (continued).

1	2	3	4	1-2-3-4
N5	C18	C19	C20	-3.2(9)
N5	C18	C19	C38	167.0(8)
C17	C18	C19	C20	177.0(8)
C17	C18	C19	C38	-12.8(13)
C38	C19	C20	C21	-169.9(8)
C38	C19	C20	C39	6.0(14)
C18	C19	C20	C21	0.7(9)
C18	C19	C20	C39	176.6(8)
C39	C20	C21	N5	-173.8(8)
C39	C20	C21	C22	6.(2)
C19	C20	C21	N5	1.9(10)
C19	C20	C21	C22	-178.2(9)
N5	C21	C22	N6	4.6(10)
N5	C21	C22	C23	-169.1(9)
C20	C21	C22	N6	-175.3(9)
C20	C21	C22	C23	11.(2)
N6	C22	C23	C24	-1.3(9)
N6	C22	C23	C40	178.9(8)
C21	C22	C23	C24	172.6(10)
C21	C22	C23	C40	-7.(2)
C40	C23	C24	C25	-178.3(8)
C40	C23	C24	C41	-2.3(15)
C22	C23	C24	C25	1.9(9)
C22	C23	C24	C41	178.0(8)
C25	C24	C41	C42	86.8(10)
C41	C24	C25	N6	-178.2(7)
C41	C24	C25	C26	3.6(14)
C23	C24	C25	N6	-1.9(9)
C23	C24	C25	C26	179.9(9)
C23	C24	C41	C42	-88.6(11)
N6	C25	C26	C1	9.9(13)
C24	C25	C26	C1	-172.2(8)

P-1090-M19

Supplementary Figure 1. View of $(C_{42}H_{46}N_6)Cu_2Cl_2$-$3CHCl_3$ showing the atom labelling scheme. Thermal ellipsoids are scaled to the 30% probability level. Hydrogen atoms are drawn to an arbitrary scale.

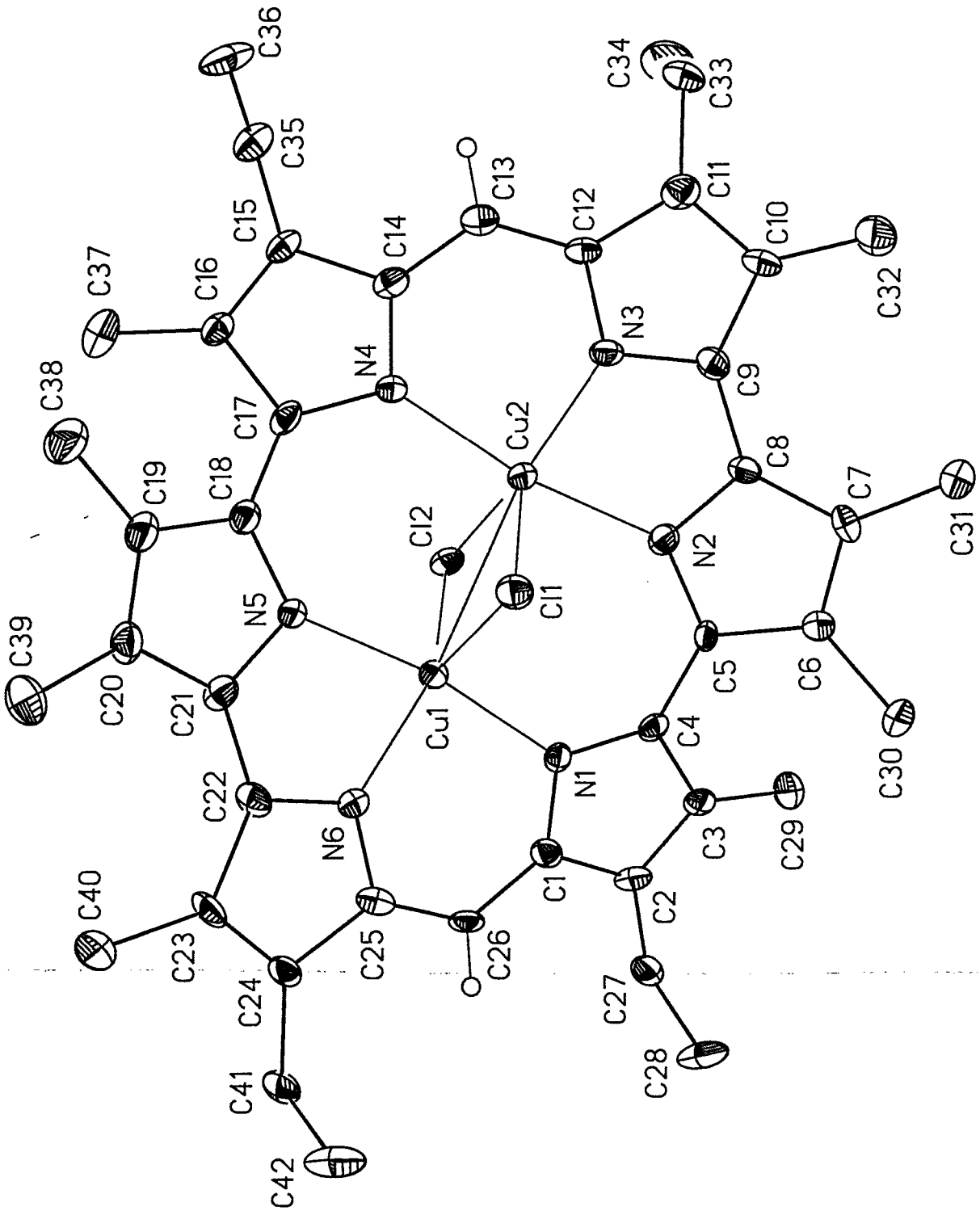
Supplementary Figure 2. Unit cell packing diagram for $(C_{42}H_{46}N_6)Cu_2Cl_2$-$3CHCl_3$. View direction is along the **b** axis.

Supplementary Figure 3. X-band EPR spectrum of *bis*[(μ-chloro)copper(II)]amethyrin **7** recorded at 77 K in frozen 2:1 CH_2Cl_2:toluene solution.

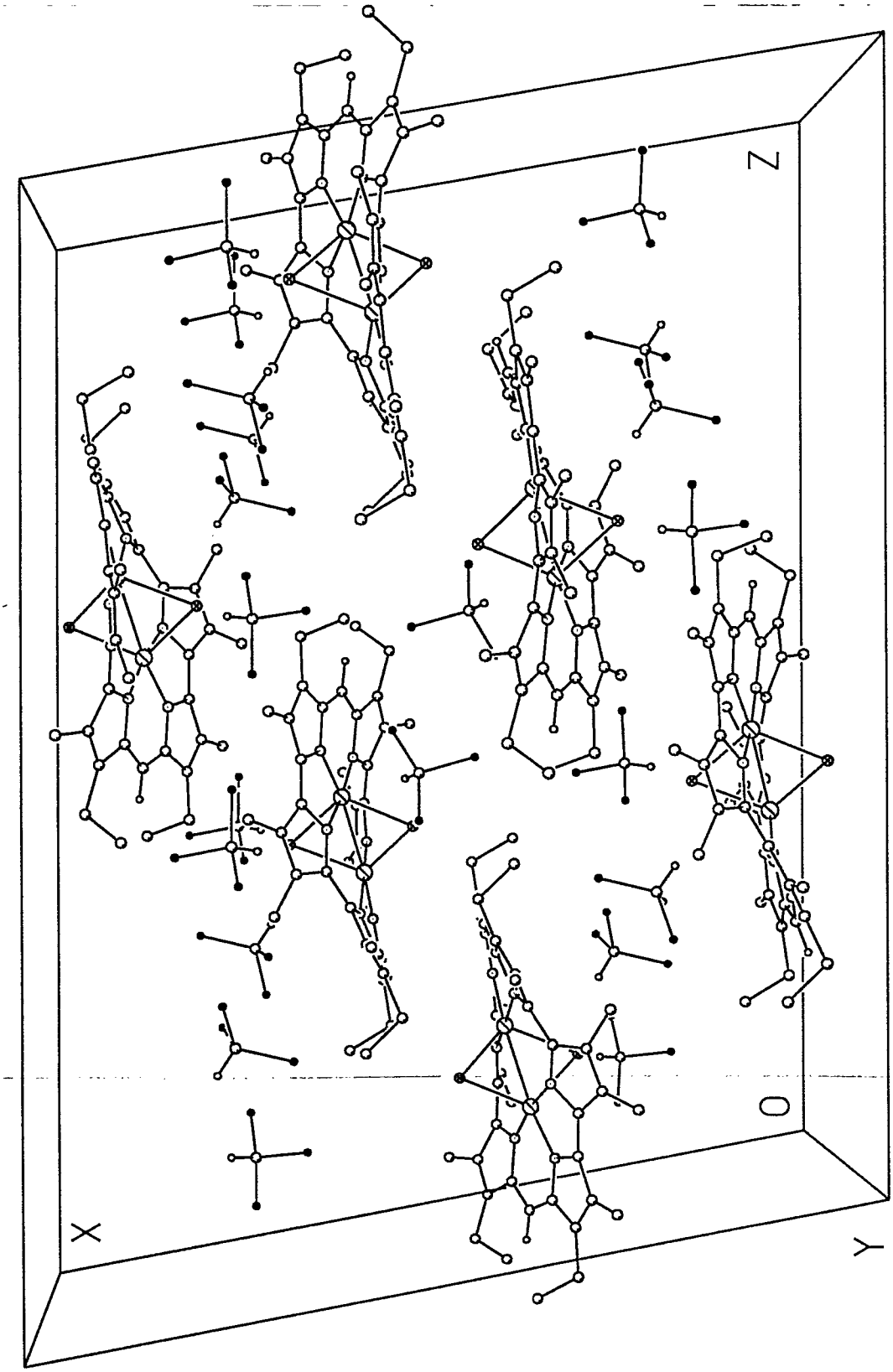
Supplementary Figure 4. Plot of χ_m^{corr} vs. T for solid **7**. The line represents the best least-squares fit of equation 1 (see text) to the experimental susceptibility data.

P-1090-m20

Supplementary Figure 1

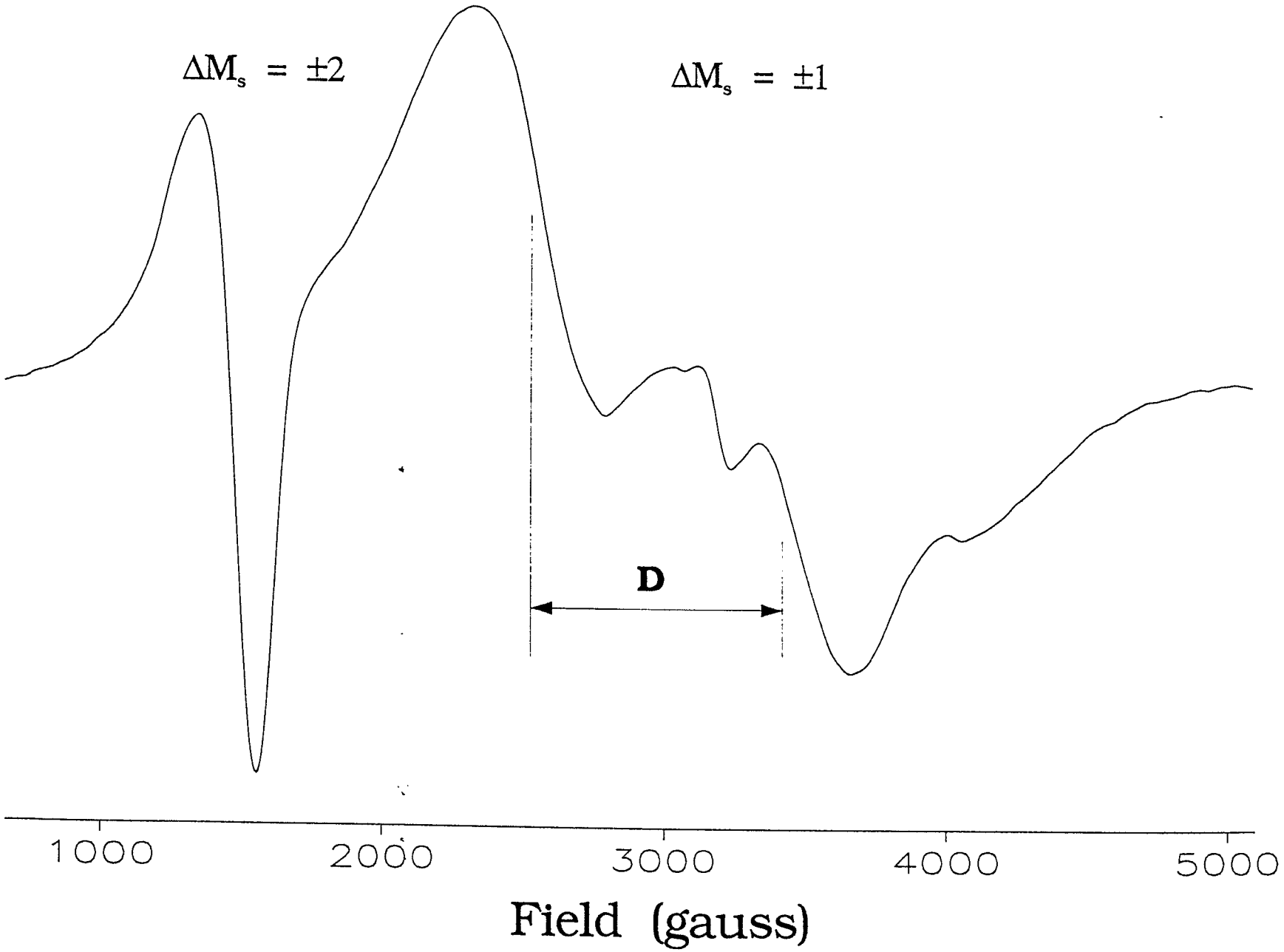


P-1090-M21



Supplementary Figure 2

Supplementary Figure 3



P-1090-M22

P-1090-M23

Supplementary Figure 4