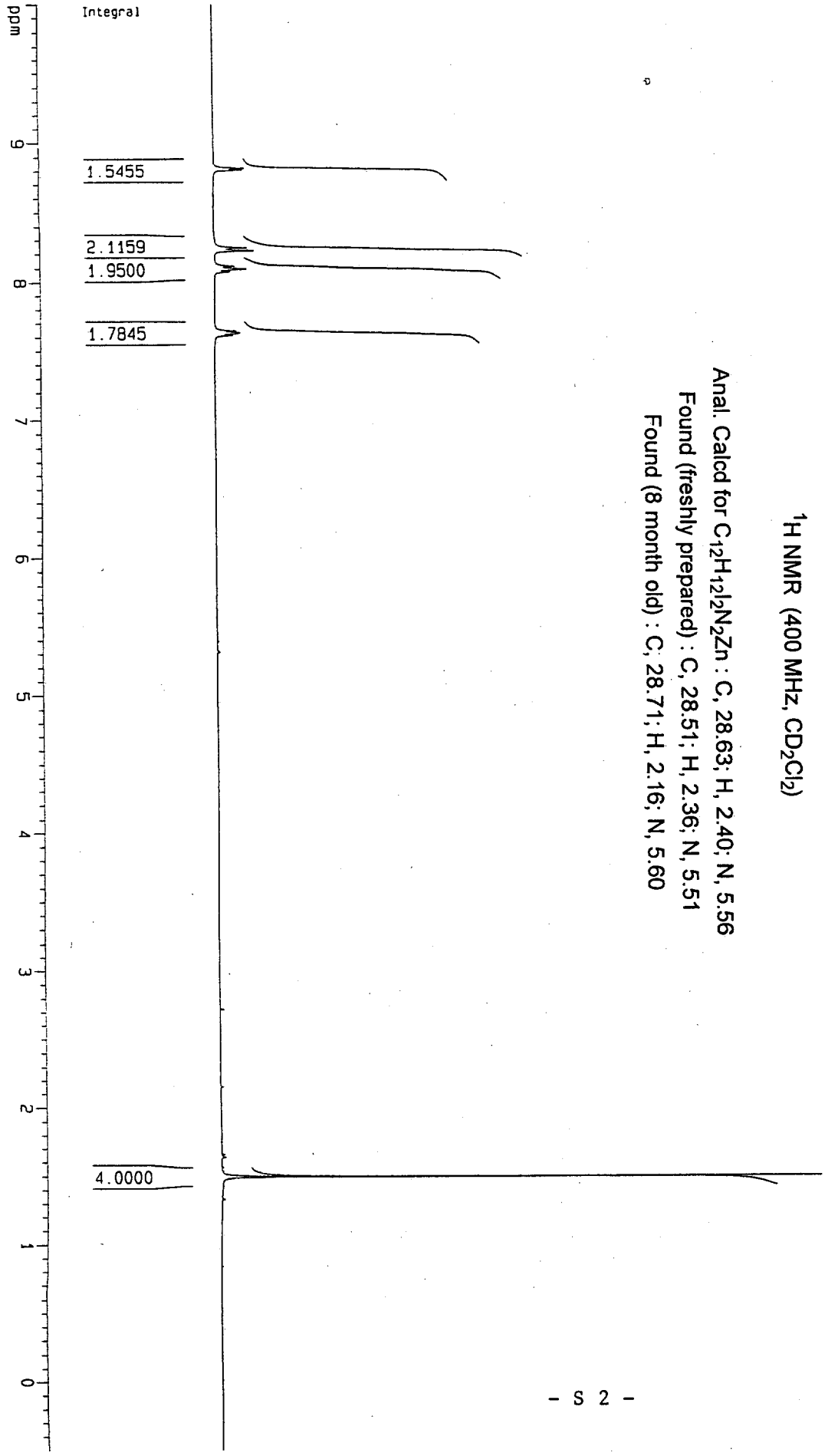
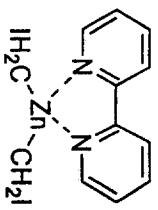
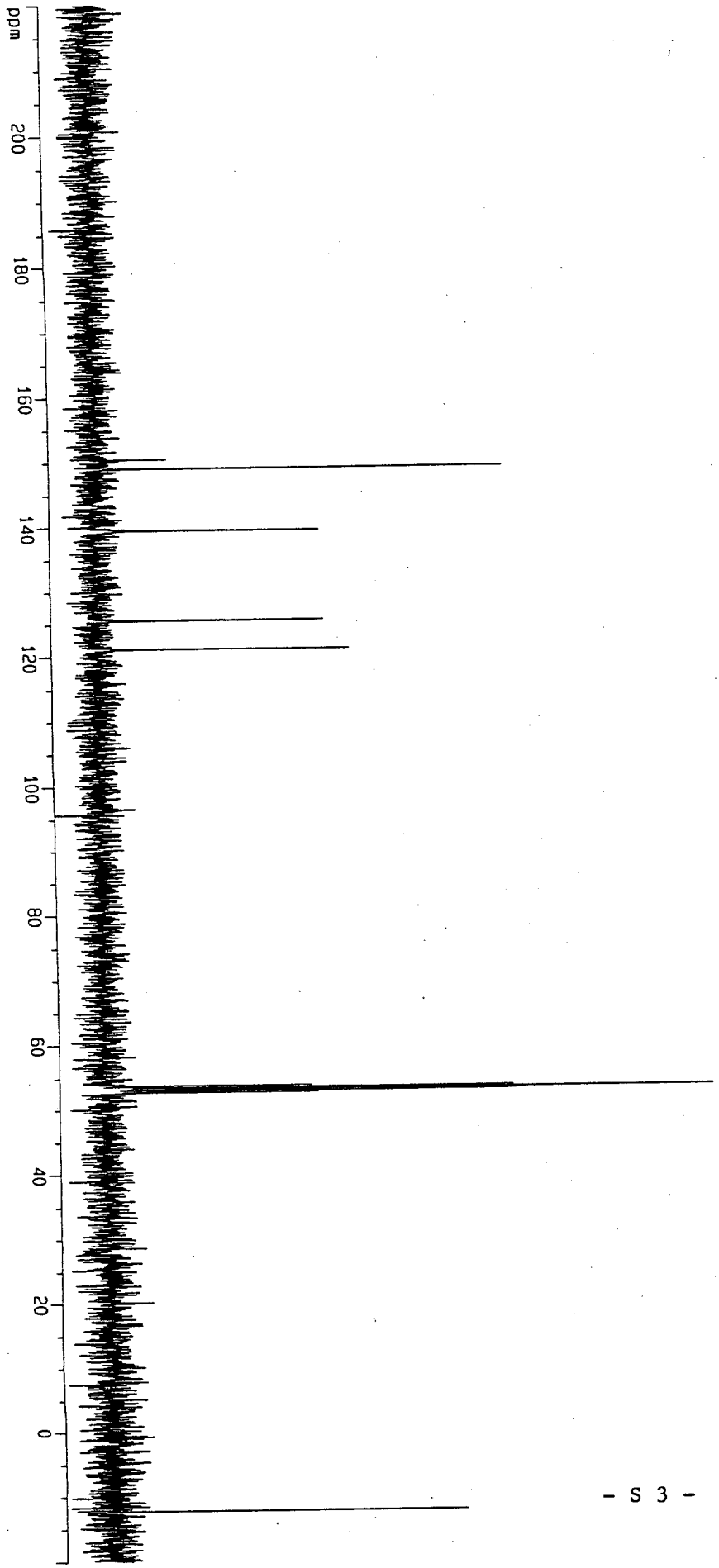




1

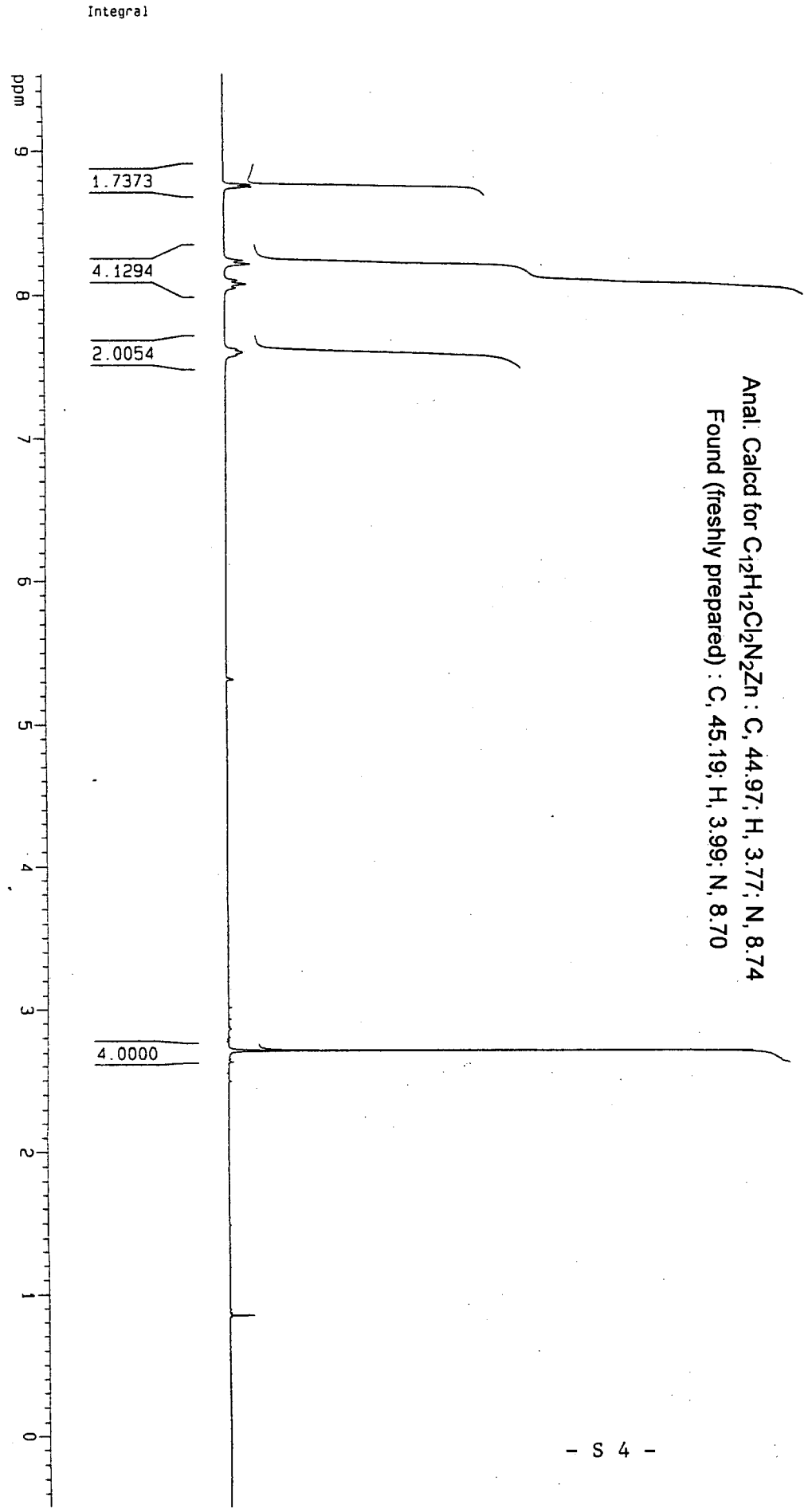
^{1}H NMR (400 MHz, CD_2Cl_2)

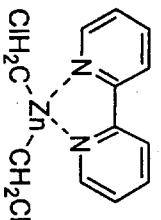
Anal. Calcd for $C_{12}H_{12}I_2N_2Zn$: C, 28.63; H, 2.40; N, 5.56
Found (freshly prepared) : C, 28.51; H, 2.36; N, 5.51
Found (8 month old) : C, 28.71; H, 2.16; N, 5.60



^{13}C NMR (100 MHz, CD_2Cl_2)

1





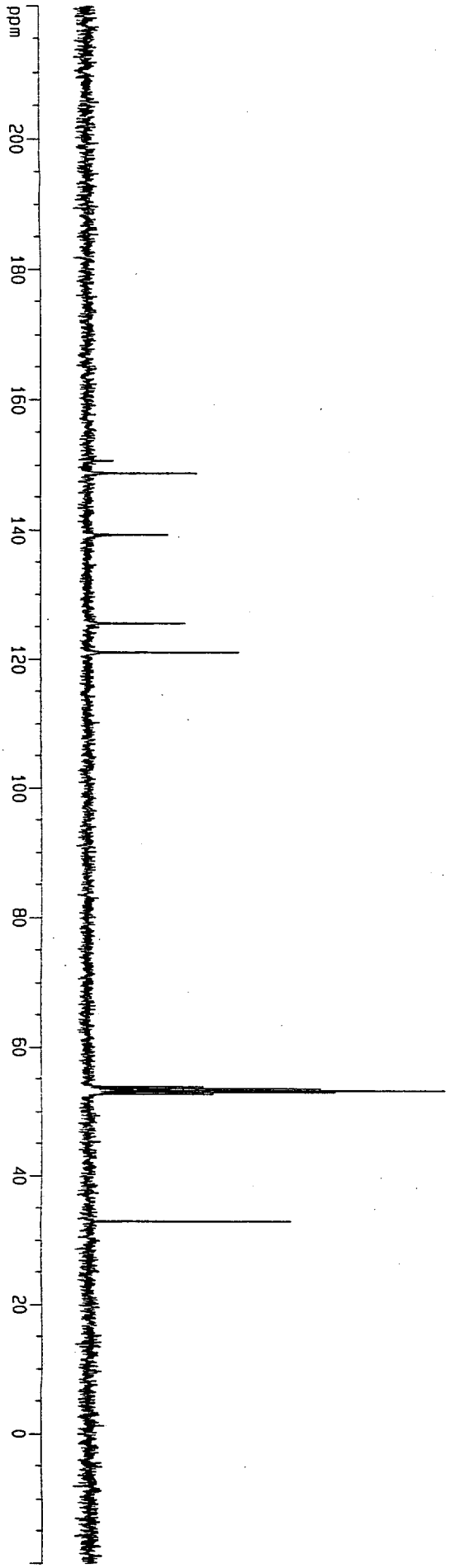
2

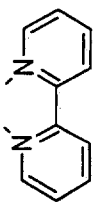
ClH_2C–Zn–CH_2Cl

^1H NMR (300 MHz, CD_2Cl_2)

Anal. Calcd for $C_{12}H_{12}Cl_2N_2Zn$: C, 44.97; H, 3.77; N, 8.74

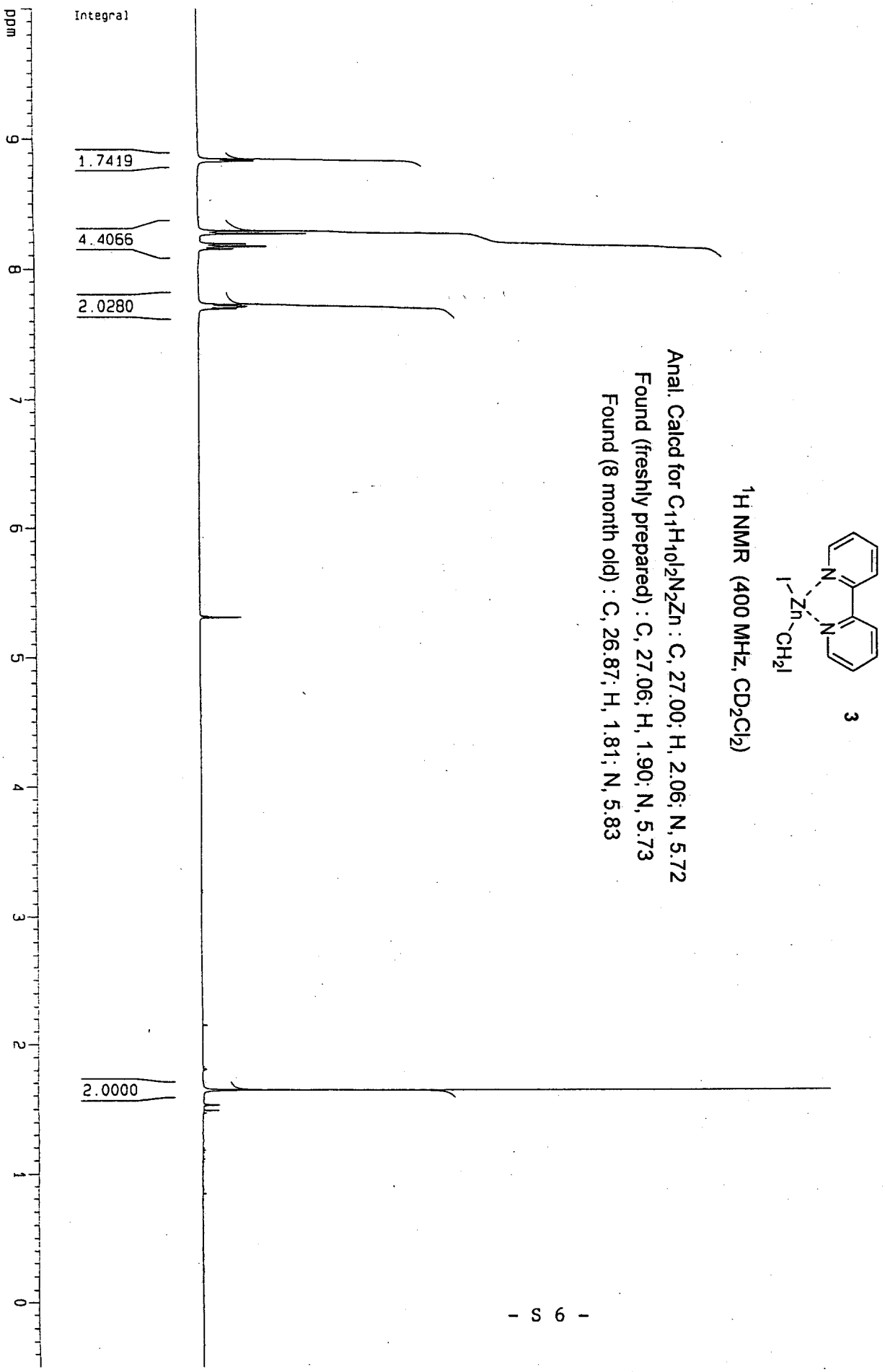
Found (freshly prepared) : C, 45.19; H, 3.99; N, 8.70





2

^{13}C NMR (100 MHz, CD_2Cl_2)



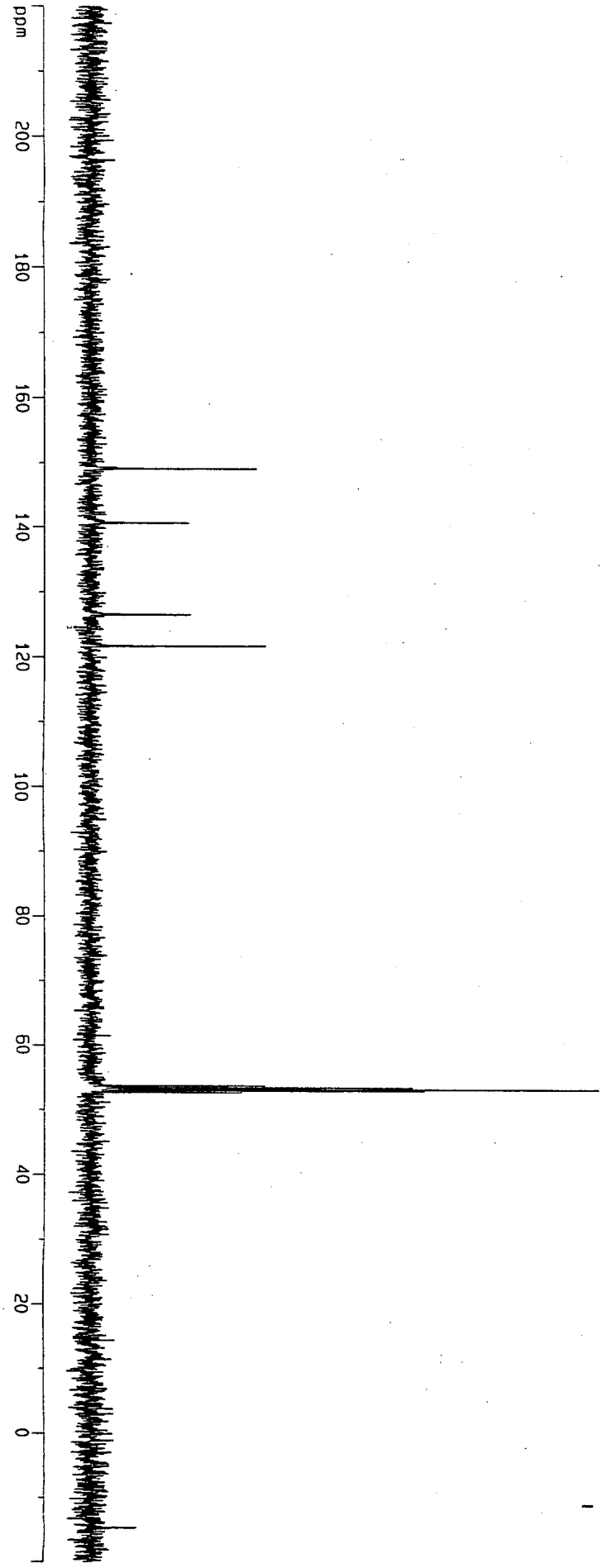
3

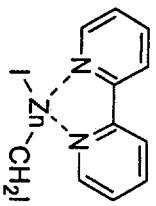
^{1}H NMR (400 MHz, CD_2Cl_2)

Anal. Calcd for $C_{11}H_{10}I_2N_2Zn$: C, 27.00; H, 2.06; N, 5.72

Found (freshly prepared) : C, 27.06; H, 1.90; N, 5.73

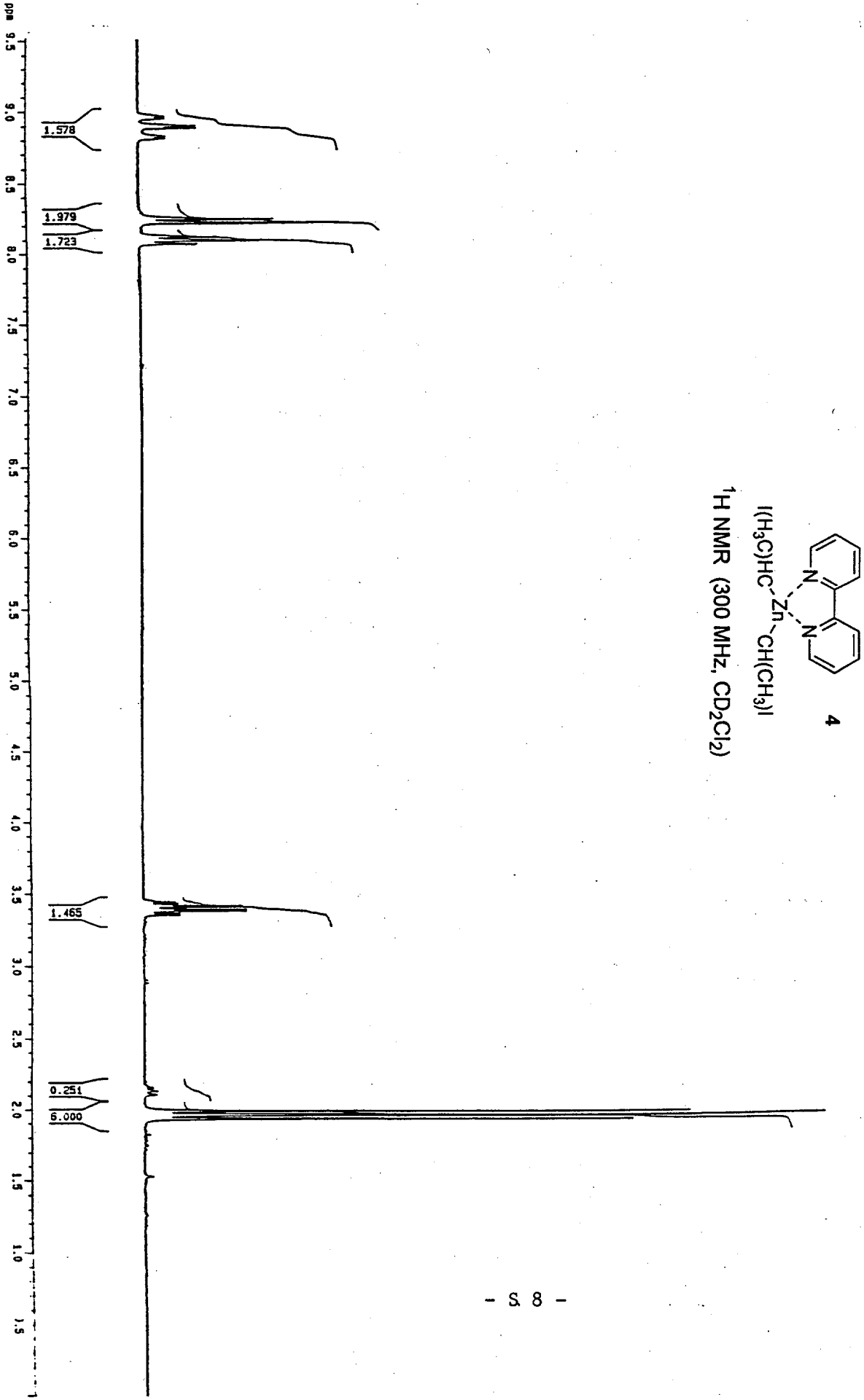
Found (8 month old) : C, 26.87; H, 1.81; N, 5.83





3

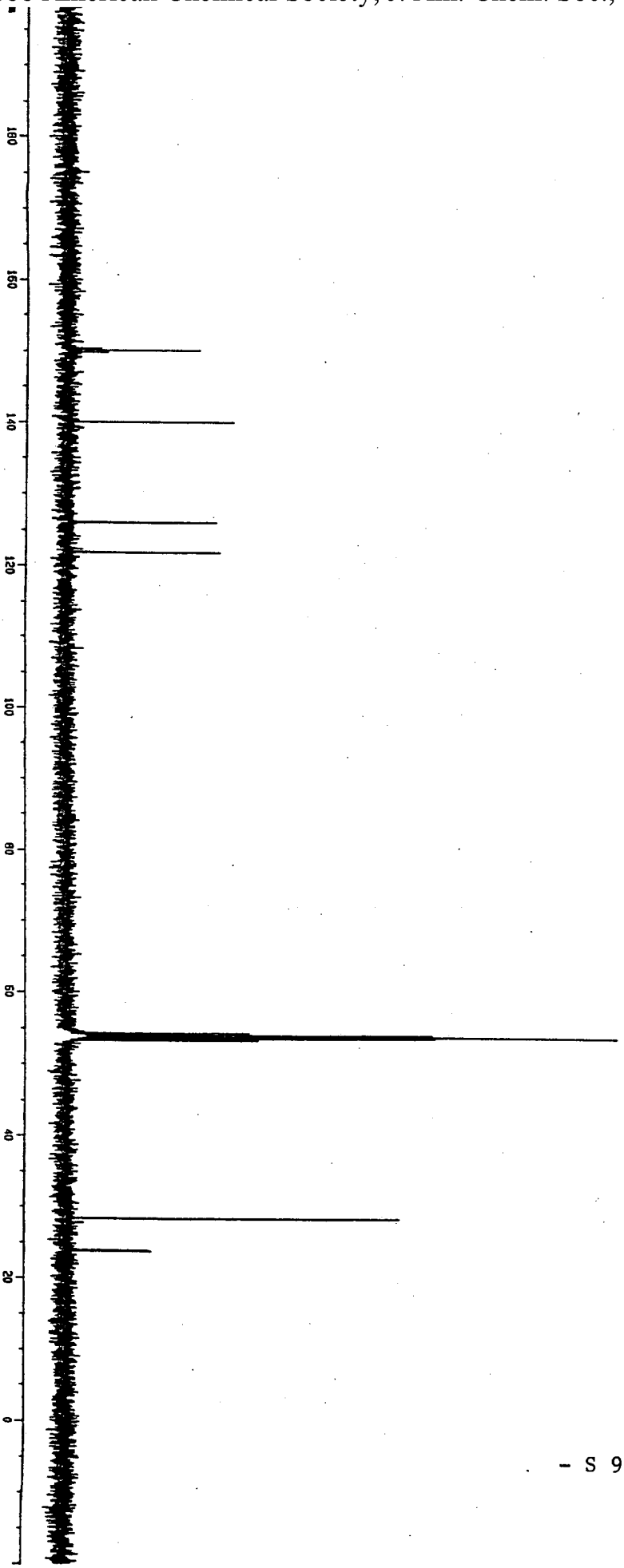
^{13}C NMR (100 MHz, CD_2Cl_2)

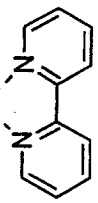


4

I(H$_3$C)HC$^-$Zn$^-$CH(CH$_3$)I

^{1}H NMR (300 MHz, CD_2Cl_2)

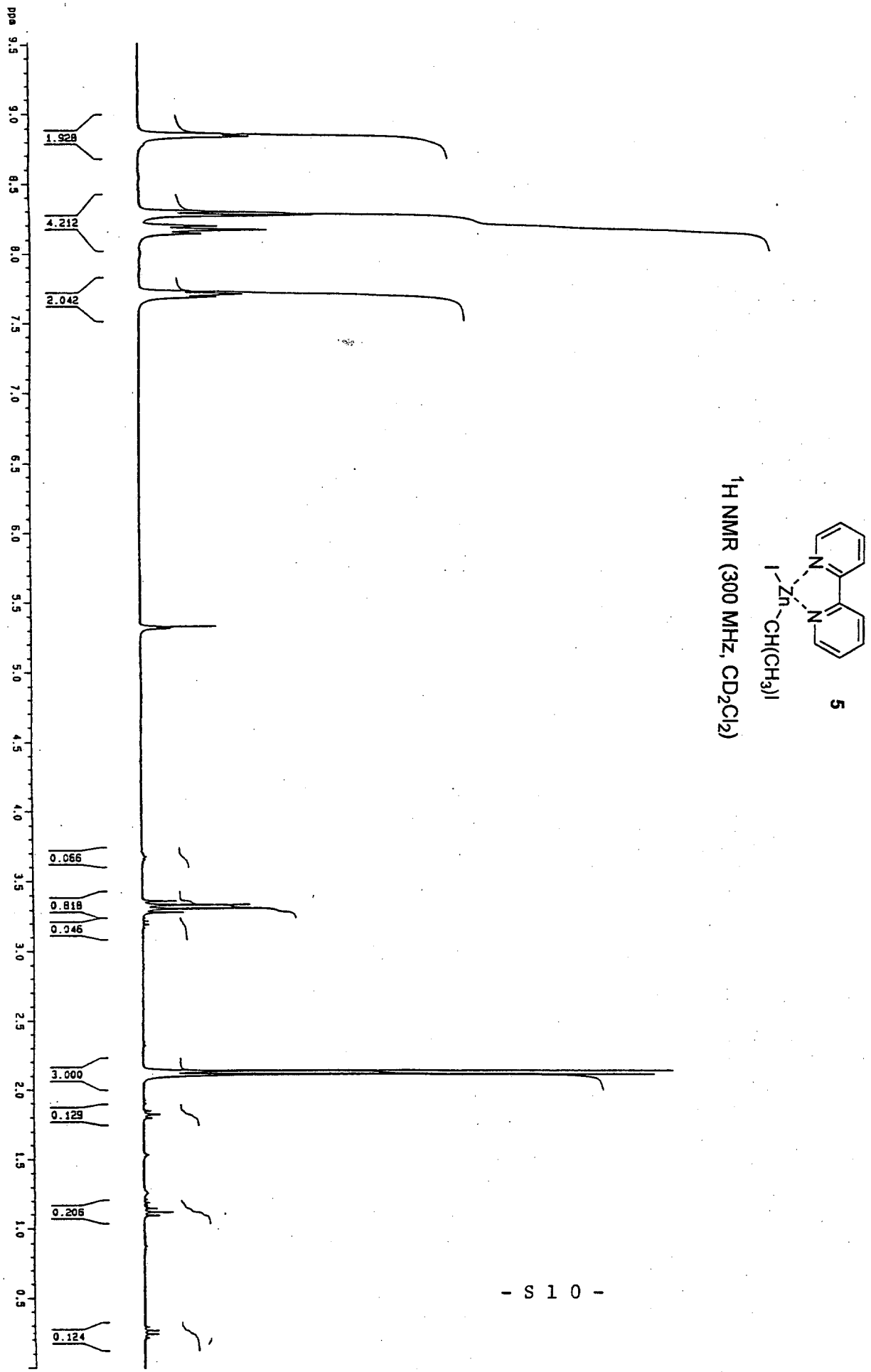




4

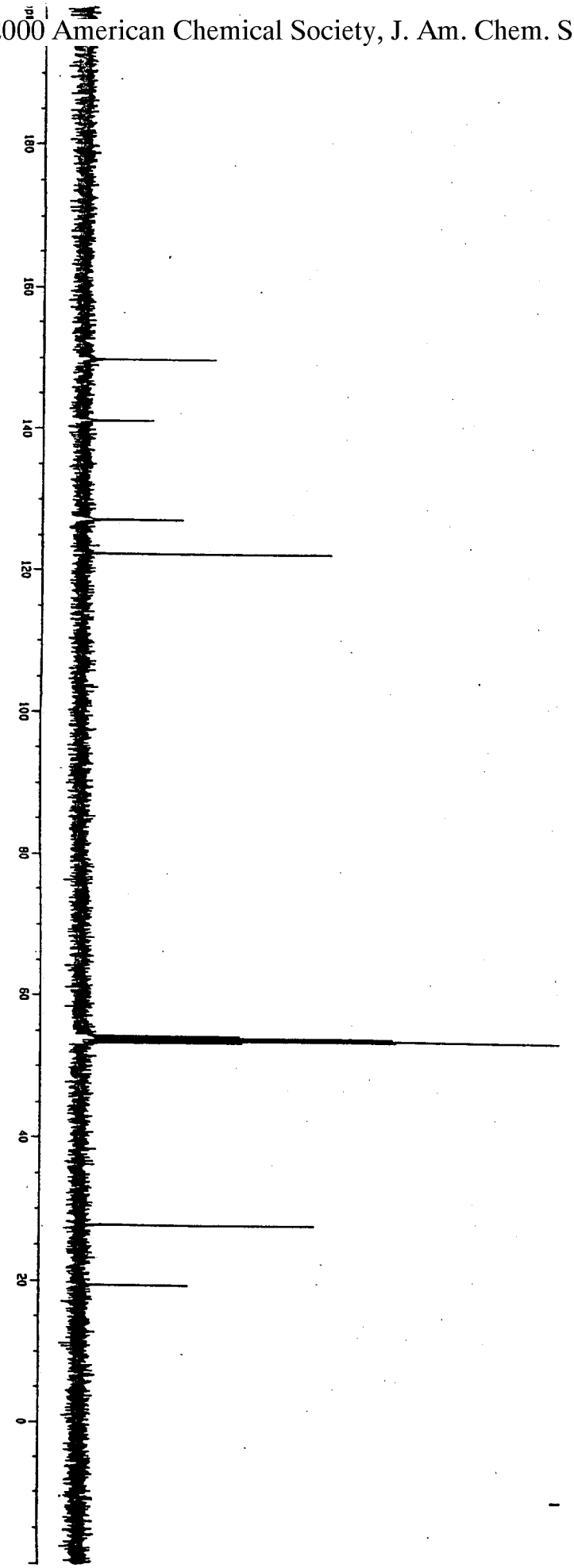
I(H$_3$C)HC–Zn–CH(CH$_3$)I

^{13}C NMR (100 MHz, CD_2Cl_2)

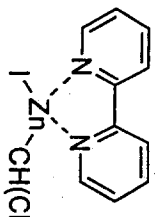


^{1}H NMR (300 MHz, CD_2Cl_2)

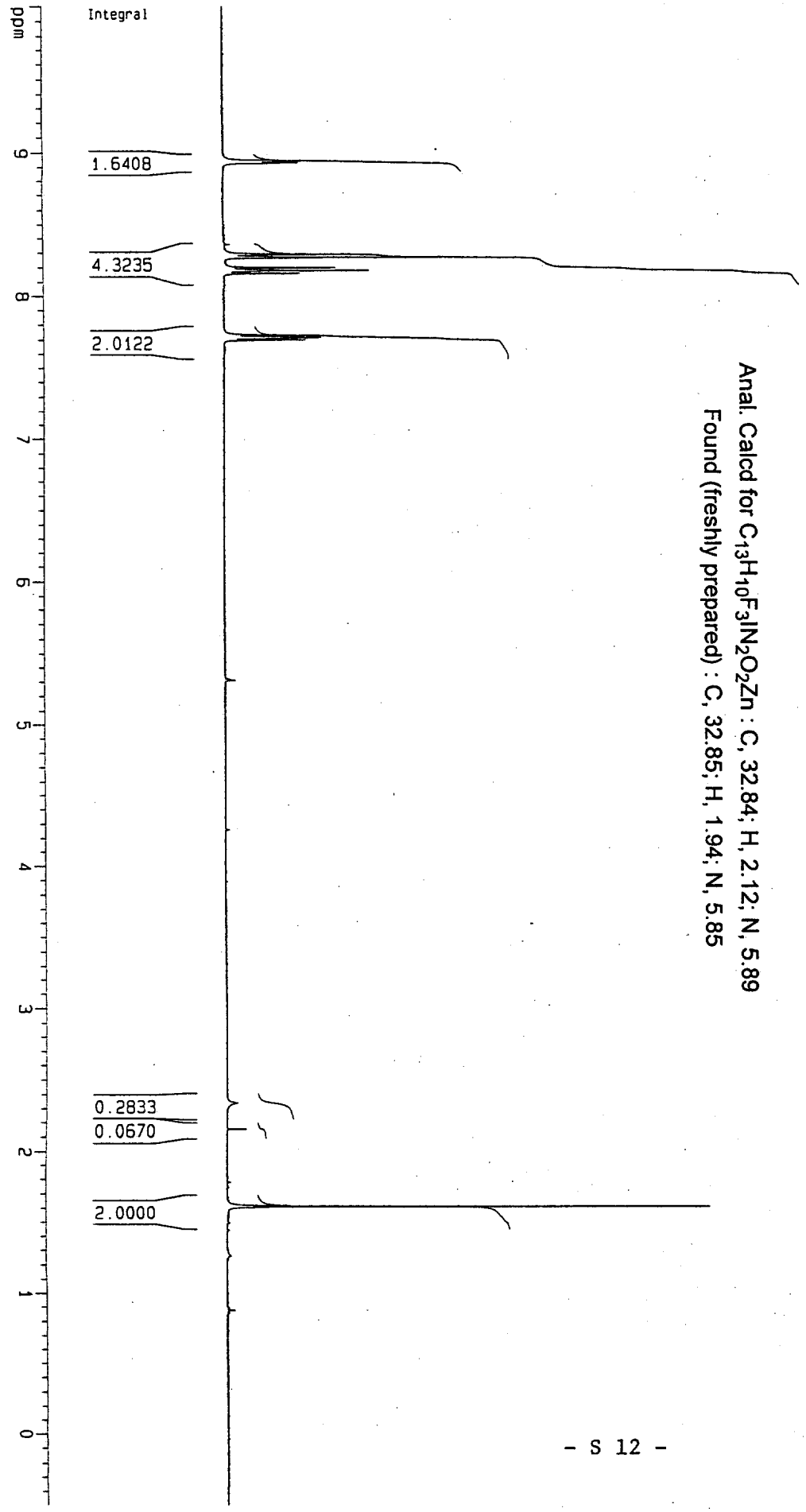
5



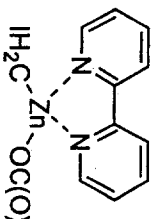
^{13}C NMR (100 MHz, CD_2Cl_2)



5



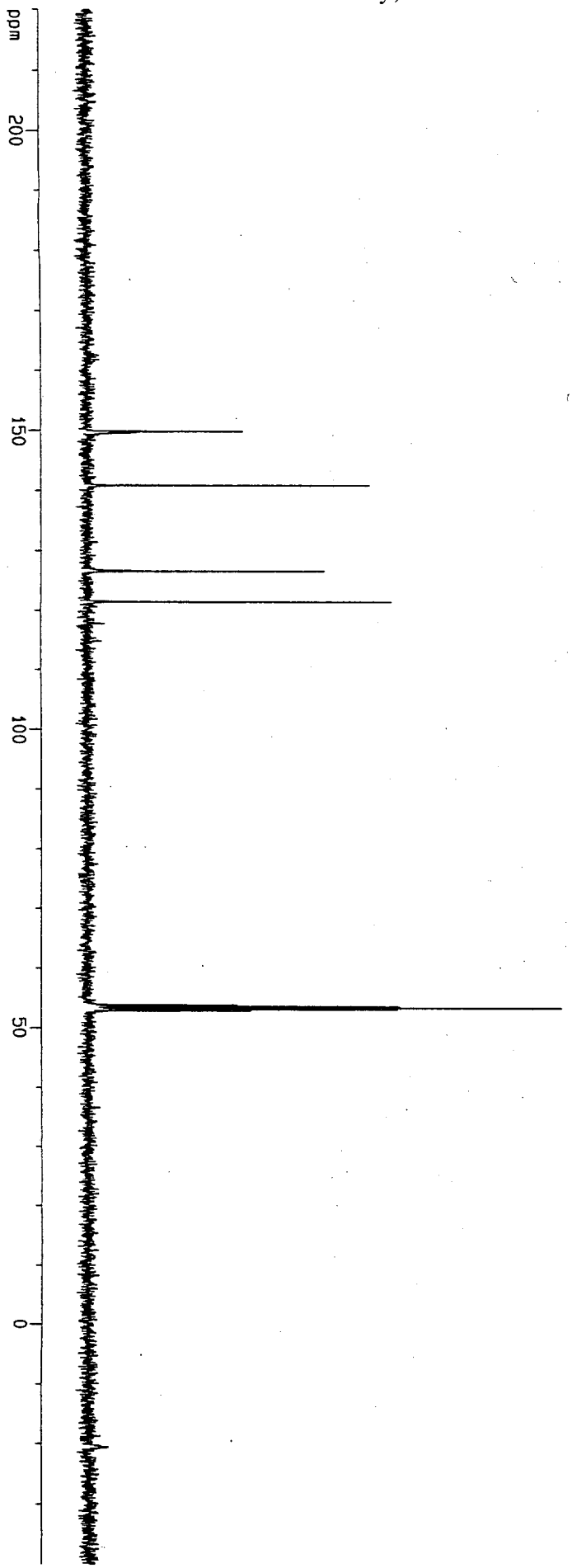
^{1}H NMR (400 MHz, CD_2Cl_2)



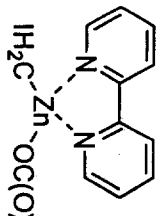
6

Anal. Calcd for $C_{13}H_{10}F_3IN_2O_2Zn$: C, 32.84; H, 2.12; N, 5.89

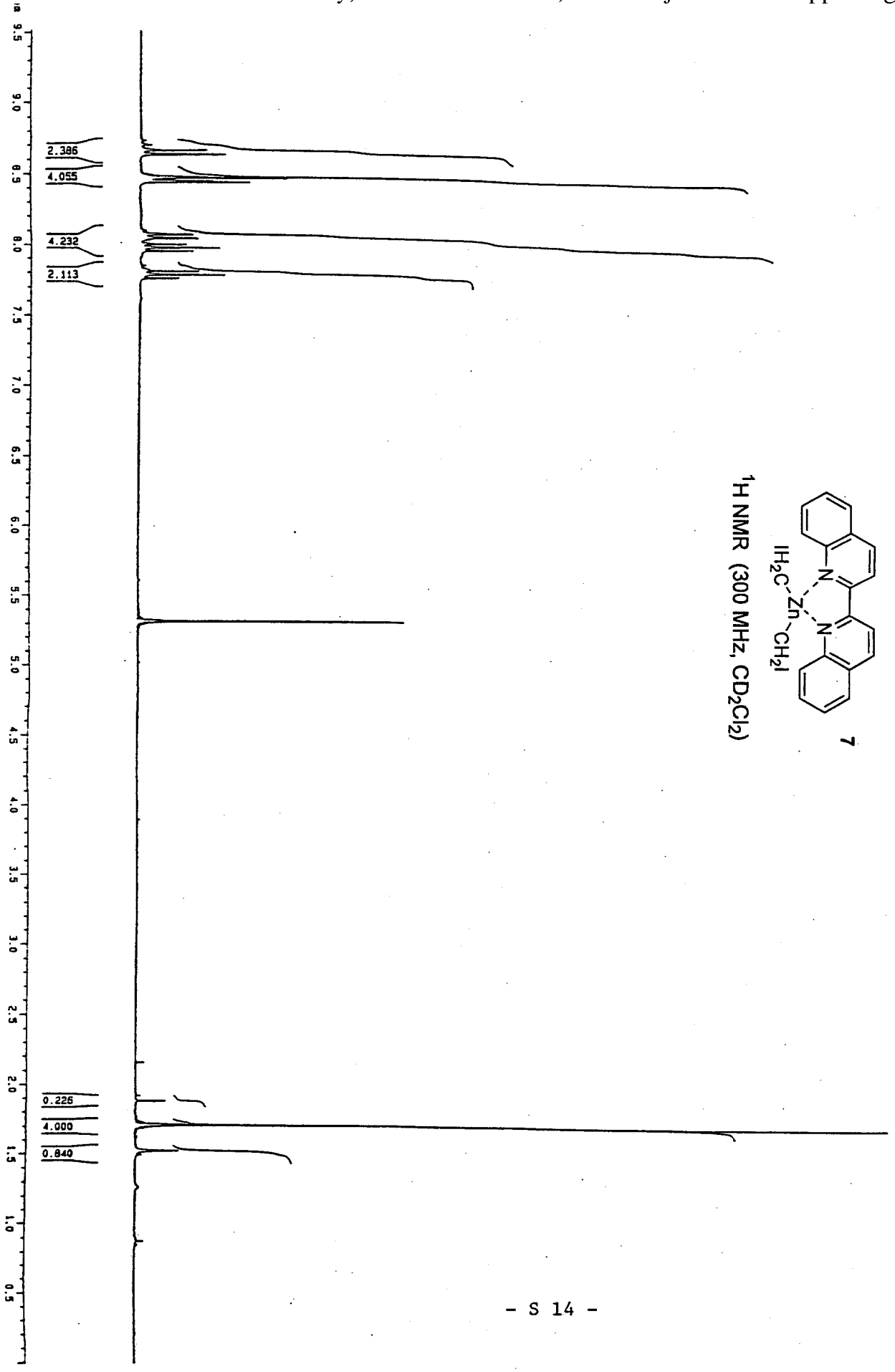
Found (freshly prepared) : C, 32.85; H, 1.94; N, 5.85



^{13}C NMR (100 MHz, CD_2Cl_2)

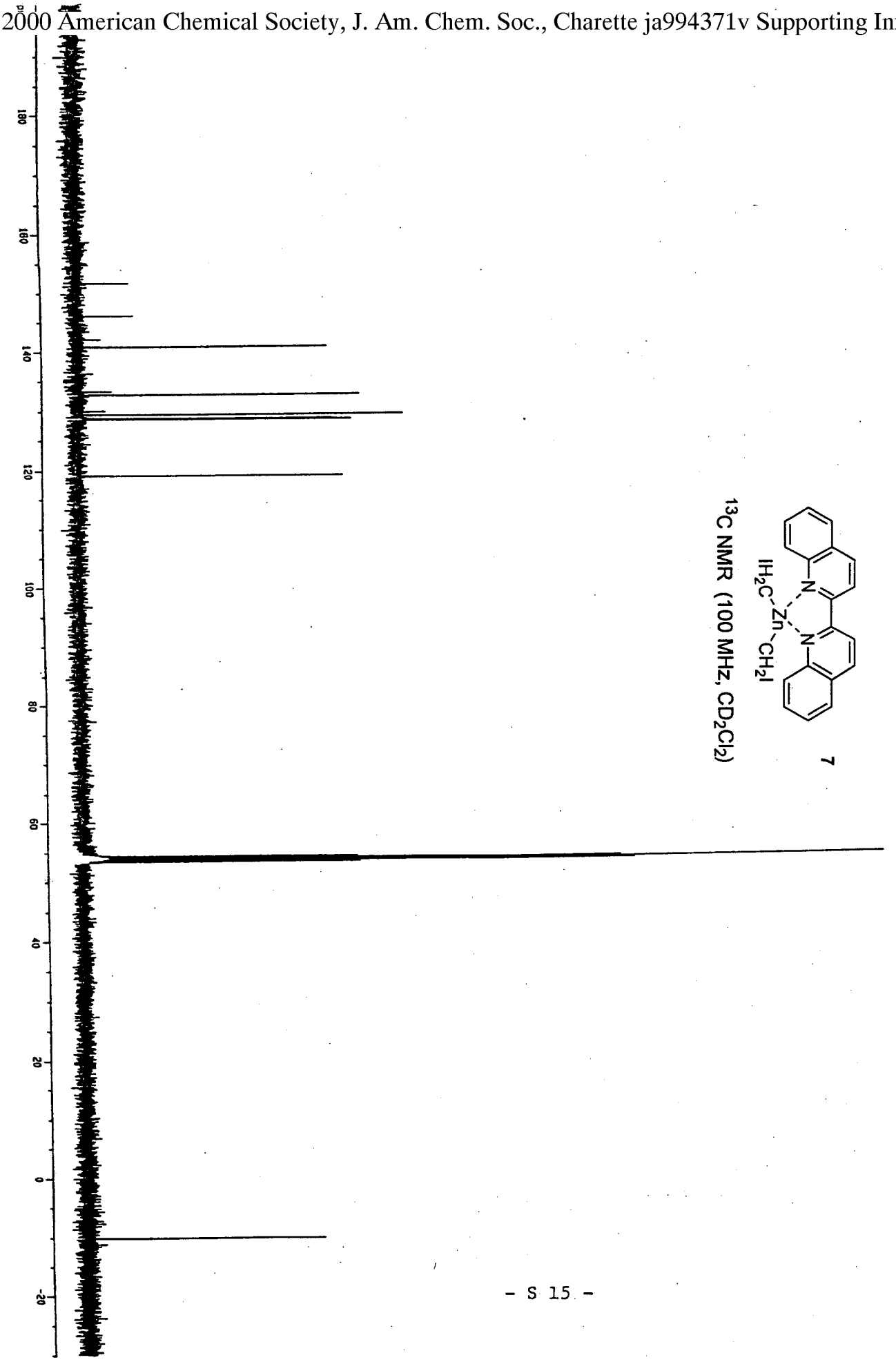


6



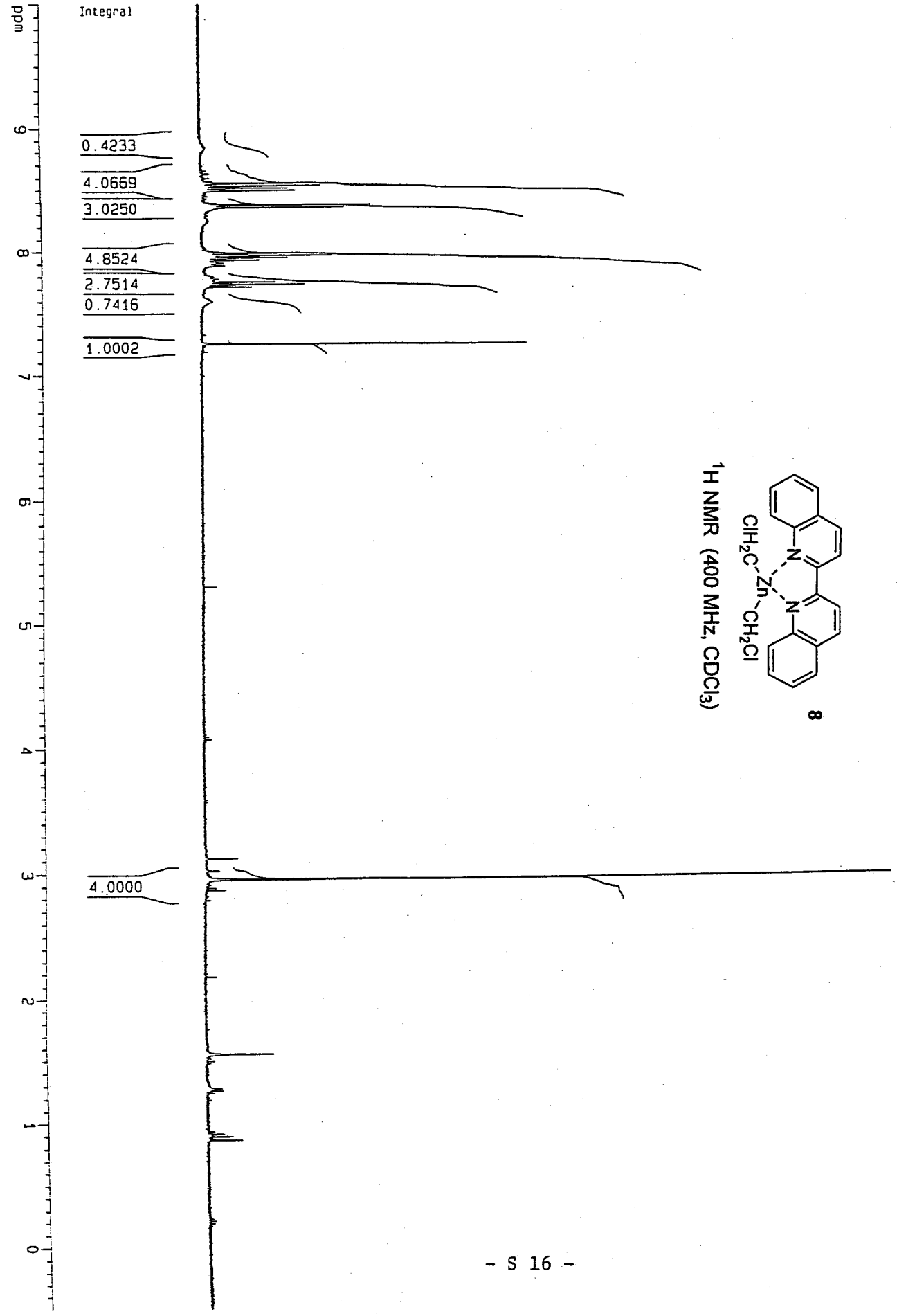
^{1}H NMR (300 MHz, CD_2Cl_2)

7



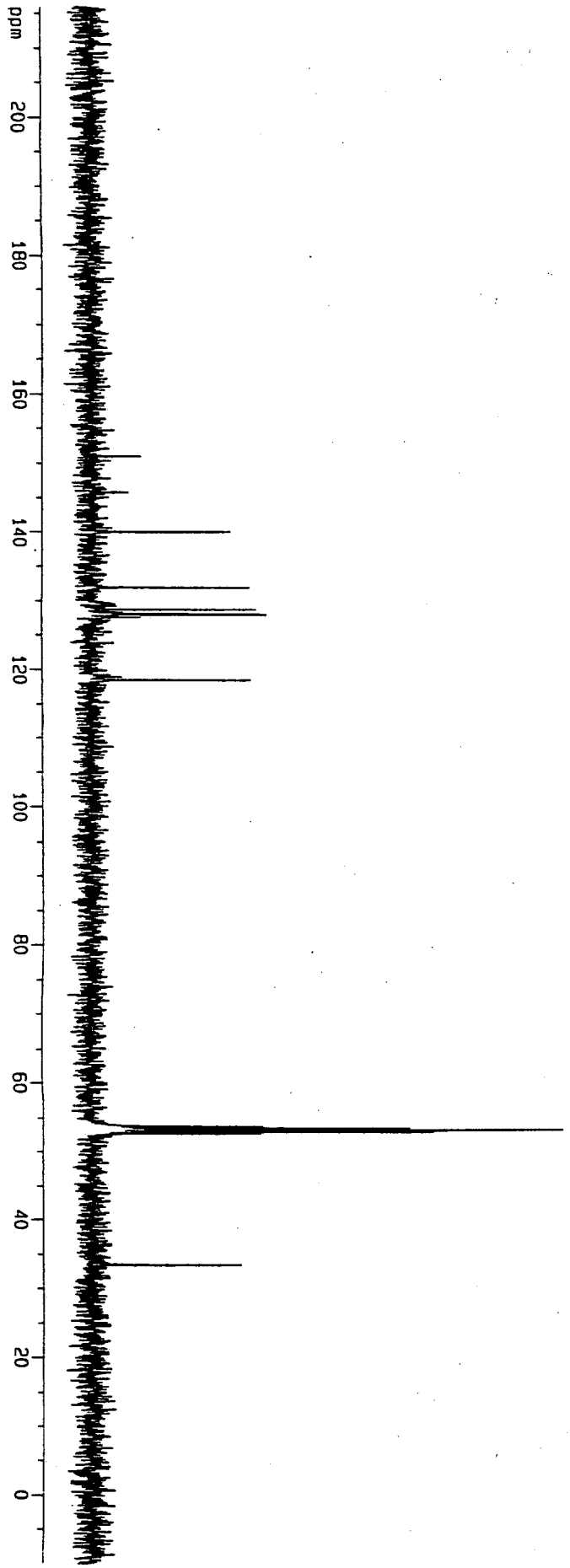
^{13}C NMR (100 MHz, CD_2Cl_2)

7

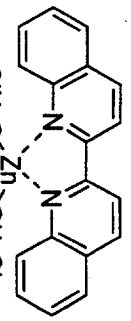


^{1}H NMR (400 MHz, $CDCl_3$)

8

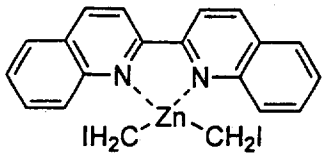


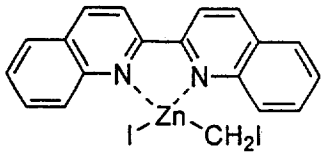
^{13}C NMR (100 MHz, CD_2Cl_2)



8

Crystal Data





Crystal data

$(C_{20}H_{16}I_2N_2Zn)_{0.9}(C_{19}H_{14}I_2N_2Zn)_{0.1}$

$M_r = 602.125$

Triclinic

$P\bar{1}$

$a = 8.819(7)$ Å

$b = 10.711(18)$ Å

$c = 11.664(15)$ Å

$\alpha = 63.53(15)°$

$\beta = 83.95(8)°$

$\gamma = 89.74(12)°$

$V = 980(2)$ Å^3

$Z = 2$

$D_x = 2.0412$ Mg m^{-3}

D_m not measured

Cu $K\alpha$ radiation

$\lambda = 1.54056$ Å

Cell parameters from 25 reflections

$\theta = 10.00–21.00°$

$\mu = 26.497$ mm^{-1}

$T = 293(2)$ K

Plate

0.42 × 0.22 × 0.07 mm

Clear red

Crystal source: synthesized by the authors, see text

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scan
Absorption correction:
by integration ABSORP in *NRCVAX*
(Gabe *et al.* 1989)
$T_{min} = 0.0233$, $T_{max} = 0.2706$
15307 measured reflections
3702 independent reflections
2791 reflections with
$>2\sigma(I)$

$R_{int} = 0.067$
$\theta_{max} = 69.78°$
$h = -10 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$
5 standard reflections
frequency: 60 min
intensity decay: no decay, variation 5.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0523$
$wR(F^2) = 0.1333$
$S = 1.078$
3702 reflections
236 parameters
H-atom parameters constrained
$w=1/[\sigma^2(F_o^2) + (0.0917P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.887$ e Å^{-3}
$\Delta\rho_{min} = -1.134$ e Å^{-3}
Extinction correction: *SHELXL*96 (Sheldrick, 1996)
Extinction coefficient: 0.0010 (2)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Zn—I1	3.477 (4)	C6—C7	1.399 (11)
Zn—I2	3.551 (7)	C7—C8	1.422 (10)
Zn—I3	2.514 (8)	C8—C9	1.333 (11)
Zn—C21	2.015 (8)	C9—C10	1.412 (10)
Zn—C22	2.082 (9)	C10—C11	1.464 (10)
Zn—N1	2.135 (7)	C11—N12	1.324 (9)
Zn—N12	2.141 (6)	C11—C20	1.415 (9)
I1—C21	2.142 (9)	N12—C13	1.367 (9)
I2—C22	2.106 (11)	C13—C14	1.403 (11)
N1—C10	1.355 (8)	C13—C18	1.410 (10)
N1—C2	1.369 (9)	C14—C15	1.357 (12)
C2—C7	1.418 (10)	C15—C16	1.396 (13)
C2—C3	1.433 (9)	C16—C17	1.319 (14)
C3—C4	1.364 (11)	C17—C18	1.444 (12)
C4—C5	1.393 (11)	C18—C19	1.393 (12)
C5—C6	1.356 (11)	C19—C20	1.368 (12)

C21—Zn—C22	125.5 (3)	N1—C10—C9	119.8 (7)
C21—Zn—N1	111.2 (3)	N1—C10—C11	115.3 (6)
C22—Zn—N1	105.6 (4)	C9—C10—C11	124.9 (6)
C21—Zn—N12	113.1 (3)	N12—C11—C20	122.3 (7)
C22—Zn—N12	113.5 (3)	N12—C11—C10	117.5 (6)
N1—Zn—N12	76.8 (2)	C20—C11—C10	120.2 (7)
C21—Zn—I3	125.4 (3)	C11—N12—C13	120.5 (6)
N1—Zn—I3	118.0 (3)	C11—N12—Zn	114.9 (5)
N12—Zn—I3	100.2 (3)	C13—N12—Zn	124.5 (5)
C10—N1—C2	119.4 (6)	N12—C13—C14	119.9 (6)
C10—N1—Zn	115.2 (5)	N12—C13—C18	120.2 (7)
C2—N1—Zn	125.4 (4)	C14—C13—C18	119.9 (7)
N1—C2—C7	122.3 (6)	C15—C14—C13	120.1 (8)
N1—C2—C3	118.4 (6)	C14—C15—C16	120.8 (9)
C7—C2—C3	119.3 (7)	C17—C16—C15	120.8 (9)
C4—C3—C2	118.5 (7)	C16—C17—C18	121.5 (9)
C3—C4—C5	121.7 (8)	C19—C18—C13	117.8 (7)
C6—C5—C4	120.8 (8)	C19—C18—C17	125.3 (8)
C5—C6—C7	120.4 (7)	C13—C18—C17	116.9 (8)
C6—C7—C2	119.3 (7)	C20—C19—C18	121.9 (7)
C6—C7—C8	124.1 (7)	C19—C20—C11	117.1 (7)
C2—C7—C8	116.6 (7)	Zn—C21—I1	113.5 (3)
C9—C8—C7	120.1 (7)	Zn—C22—I2	116.0 (5)
C8—C9—C10	121.8 (7)		

C21—Zn—N1—C10	112.9 (5)	C20—C11—N12—Zn	−173.4 (5)
C22—Zn—N1—C10	−108.2 (5)	C10—C11—N12—Zn	6.4 (7)
N12—Zn—N1—C10	3.0 (4)	C21—Zn—N12—C11	−112.7 (5)
I3—Zn—N1—C10	−91.7 (5)	C22—Zn—N12—C11	96.4 (6)
C21—Zn—N1—C2	−68.9 (6)	N1—Zn—N12—C11	−5.0 (4)
C22—Zn—N1—C2	70.0 (6)	I3—Zn—N12—C11	111.6 (5)
N12—Zn—N1—C2	−178.8 (5)	C21—Zn—N12—C13	71.2 (6)
I3—Zn—N1—C2	86.5 (6)	C22—Zn—N12—C13	−79.7 (6)
C10—N1—C2—C7	−1.5 (9)	N1—Zn—N12—C13	178.9 (6)
Zn—N1—C2—C7	−179.7 (5)	I3—Zn—N12—C13	−64.5 (6)
C10—N1—C2—C3	179.3 (6)	C11—N12—C13—C14	174.5 (7)
Zn—N1—C2—C3	1.2 (8)	Zn—N12—C13—C14	−9.6 (9)
N1—C2—C3—C4	−179.9 (6)	C11—N12—C13—C18	−3.7 (10)
C7—C2—C3—C4	1.0 (10)	Zn—N12—C13—C18	172.1 (5)
C2—C3—C4—C5	0.2 (11)	N12—C13—C14—C15	179.9 (8)
C3—C4—C5—C6	−1.1 (13)	C18—C13—C14—C15	−1.8 (12)
C4—C5—C6—C7	0.7 (12)	C13—C14—C15—C16	0.6 (14)
C5—C6—C7—C2	0.4 (11)	C14—C15—C16—C17	−1.0 (16)
C5—C6—C7—C8	179.4 (7)	C15—C16—C17—C18	2.6 (16)
N1—C2—C7—C6	179.6 (6)	N12—C13—C18—C19	1.2 (10)
C3—C2—C7—C6	−1.3 (10)	C14—C13—C18—C19	−177.1 (7)
N1—C2—C7—C8	0.5 (10)	N12—C13—C18—C17	−178.5 (7)
C3—C2—C7—C8	179.7 (6)	C14—C13—C18—C17	3.3 (11)
C6—C7—C8—C9	−178.9 (7)	C16—C17—C18—C19	176.6 (9)
C2—C7—C8—C9	0.1 (11)	C16—C17—C18—C13	−3.7 (14)
C7—C8—C9—C10	0.3 (12)	C13—C18—C19—C20	2.3 (12)
C2—N1—C10—C9	1.9 (9)	C17—C18—C19—C20	−178.0 (8)
Zn—N1—C10—C9	−179.8 (5)	C18—C19—C20—C11	−3.2 (12)
C2—N1—C10—C11	−179.0 (5)	N12—C11—C20—C19	0.6 (11)
Zn—N1—C10—C11	−0.7 (7)	C10—C11—C20—C19	−179.1 (7)
C8—C9—C10—N1	−1.3 (11)	C22—Zn—C21—I1	165.6 (4)
C8—C9—C10—C11	179.7 (7)	N1—Zn—C21—I1	−65.4 (4)
N1—C10—C11—N12	−3.8 (9)	N12—Zn—C21—I1	18.8 (5)
C9—C10—C11—N12	175.2 (6)	I3—Zn—C21—I1	141.4 (4)
N1—C10—C11—C20	176.0 (6)	C21—Zn—C22—I2	−98.3 (5)
C9—C10—C11—C20	−5.0 (10)	N1—Zn—C22—I2	130.4 (4)
C20—C11—N12—C13	2.8 (10)	N12—Zn—C22—I2	48.3 (5)
C10—C11—N12—C13	−177.4 (6)	I3—Zn—C22—I2	−1.5 (6)

Data collection: CAD-4 software (Enraf–Nonius, 1989). Cell refinement: CAD-4 software (Enraf–Nonius, 1989). Data reduction: NRC-2, NRC-2A (Ahmed *et al.* 1973). Program(s) used to solve structure: *SHELXS*96 (Sheldrick, 1990). Program(s) used to refine structure: *NRCVAX* (Gabe *et al.* 1989) and *SHELXL*96 (Sheldrick, 1996). Molecular graphics: *ORTEP*II (Johnson (1976) in *NRCVAX* (Gabe *et al.*(1989)). Software used to prepare material for publication: *NRCVAX* (Gabe *et al.*(1989) and *SHELXL*96 (Sheldrick (1996)).

References

Ahmed, F. R., Hall, S. R., Pippy, M. E. & Huber, C. P. (1973). NRC Crystallographic Computer Programs for the IBM/360. Accession Nos. 133–147 in *J. Appl. Cryst.* 6, 309–346.

Enraf–Nonius (1989). CAD-4 Software. Version 5.0. Enraf–Nonius, Delft, The Netherlands.

Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* 22, 384–387.

International Tables for Crystallography (1992). Vol. C. Tables 4.2.6.8 and 6.1.1. 4, Dordrecht: Kluwer Academic Publishers.

Johnson, C. K. (1976). *ORTEP*II - A Fortran Thermal Ellipsoid Plot Program, Technical Report ORNL-5138. Oak Ridge National Laboratory, Tenessee, USA.

Sheldrick, G. M. (1990). *SHELXS*96. Program for the Solution *of Crystal Structures.* University of Göttingen, Germany.

Sheldrick, G. M. (1996). *SHELXL*96. Program for the Refinement *of Crystal Structures.* University of Göttingen, Germany.

Spek, A. L. (1995). *PLATON* Molecular Geometry Program, July 1995 version. University of Utrecht, Utrecht, Holland.

Fig. 1 *ORTEP* (Johnson, 1976) drawing of the molecule. Ellipsoids correspond to 40% probability.

Space group confirmed by *PLATON* program (Spek, 1995). Data reduction performed using a locally modified version of the NRC-2 program (Ahmed *et al.* 1973). The structure was solved by direct method using *SHELXS*96 (Sheldrick, 1990) and difmap synthesis using *NRCVAX* (Gabe *et al.*(1989) and *SHELXL*96 (Sheldrick, 1996). All non-H atoms anisotropic, H atoms isotropic. H atoms constrained to the parent site using a riding model; *SHELXL*96 defaults, C—H 0.93 to 0.97 Å. The isotropic factors, U_{iso} , were adjusted to 20% higher value of the parent site. A final verification of possible voids was performed using the VOID routine of the *PLATON* program (Spek, 1995). A total of 5 peaks of 1.69–1.02 e/*A^3 were found located at <1.10*A from the heavy atoms locations. The general background was found to be < 0.52 e/*A^3.

Data collection: CAD-4 software (Enraf–Nonius, 1989). Cell refinement: CAD-4 software (Enraf–Nonius, 1989). Data reduction: NRC-2, NRC-2A (Ahmed *et al.* 1973). Program(s) used to solve structure: *SHELXS*96 (Sheldrick, 1990). Program(s) used to refine structure: *NRCVAX* (Gabe *et al.* 1989) and *SHELXL*96 (Sheldrick, 1996). Molecular graphics: *ORTEP*II (Johnson (1976) in *NRCVAX* (Gabe *et al.*(1989)). Software used to prepare material for publication: *NRCVAX* (Gabe *et al.*(1989) and *SHELXL*96 (Sheldrick (1996)).

Table *S1*. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	Occupancy	*x*	*y*	*z*	U_{eq}
Zn	1	0.65631 (12)	0.47277 (9)	0.19811 (8)	0.0530 (3)
I1	1	0.99386 (7)	0.29955 (6)	0.21527 (5)	0.0703 (2)
I2	0.90	0.52993 (8)	0.81377 (6)	0.01838 (5)	0.0715 (2)
I3	0.10	0.5134 (9)	0.6862 (9)	0.0738 (6)	0.0822 (17)
N1	1	0.5617 (6)	0.3338 (5)	0.3896 (5)	0.0478 (12)
C2	1	0.4563 (8)	0.2266 (6)	0.4220 (6)	0.0465 (14)
C3	1	0.4055 (9)	0.2020 (7)	0.3208 (7)	0.0555 (16)
H3	1	0.4435	0.2574	0.2352	0.067
C4	1	0.3003 (9)	0.0953 (8)	0.3530 (8)	0.0640 (19)
H4	1	0.2668	0.0783	0.2880	0.077
C5	1	0.2416 (10)	0.0113 (8)	0.4806 (8)	0.070 (2)
H5	1	0.1687	−0.0596	0.4991	0.083
C6	1	0.2895 (9)	0.0315 (7)	0.5780 (8)	0.0643 (19)
H6	1	0.2501	−0.0261	0.6627	0.077
C7	1	0.3978 (9)	0.1387 (7)	0.5517 (7)	0.0570 (17)
C8	1	0.4531 (10)	0.1680 (8)	0.6477 (7)	0.0615 (19)
H8	1	0.4185	0.1132	0.7343	0.074
C9	1	0.5547 (10)	0.2737 (8)	0.6140 (7)	0.0609 (18)
H9	1	0.5901	0.2913	0.6780	0.073
C10	1	0.6099 (8)	0.3598 (7)	0.4838 (6)	0.0476 (14)
C11	1	0.7206 (8)	0.4778 (7)	0.4395 (7)	0.0529 (16)
N12	1	0.7693 (7)	0.5420 (6)	0.3147 (5)	0.0503 (12)
C13	1	0.8772 (8)	0.6495 (7)	0.2675 (7)	0.0528 (16)
C14	1	0.9372 (11)	0.7085 (8)	0.1372 (8)	0.070 (2)
H14	1	0.9036	0.6744	0.0831	0.085
C15	1	1.0442 (11)	0.8154 (9)	0.0899 (9)	0.077 (2)
H15	1	1.0828	0.8546	0.0032	0.092
C16	1	1.0970 (12)	0.8672 (10)	0.1698 (11)	0.087 (3)
H16	1	1.1714	0.9395	0.1360	0.105
C17	1	1.0424 (12)	0.8147 (10)	0.2926 (11)	0.083 (3)
H17	1	1.0762	0.8534	0.3432	0.099
C18	1	0.9313 (9)	0.6986 (8)	0.3503 (8)	0.0599 (17)
C19	1	0.8735 (10)	0.6324 (9)	0.4802 (8)	0.069 (2)
H19	1	0.9050	0.6655	0.5356	0.082
C20	1	0.7715 (9)	0.5201 (8)	0.5284 (7)	0.0591 (17)
H20	1	0.7371	0.4735	0.6160	0.071
C21	1	0.7938 (10)	0.3732 (9)	0.1201 (7)	0.066 (2)
H21A	1	0.8248	0.4362	0.0301	0.080
H21B	1	0.7366	0.2943	0.1232	0.080
C22	0.90	0.4791 (11)	0.5969 (10)	0.1125 (9)	0.060 (2)
H22A	0.90	0.3938	0.5781	0.1786	0.072
H22B	0.90	0.4460	0.5688	0.0504	0.072

Table *S2*. *Anisotropic displacement parameters* (Å²)

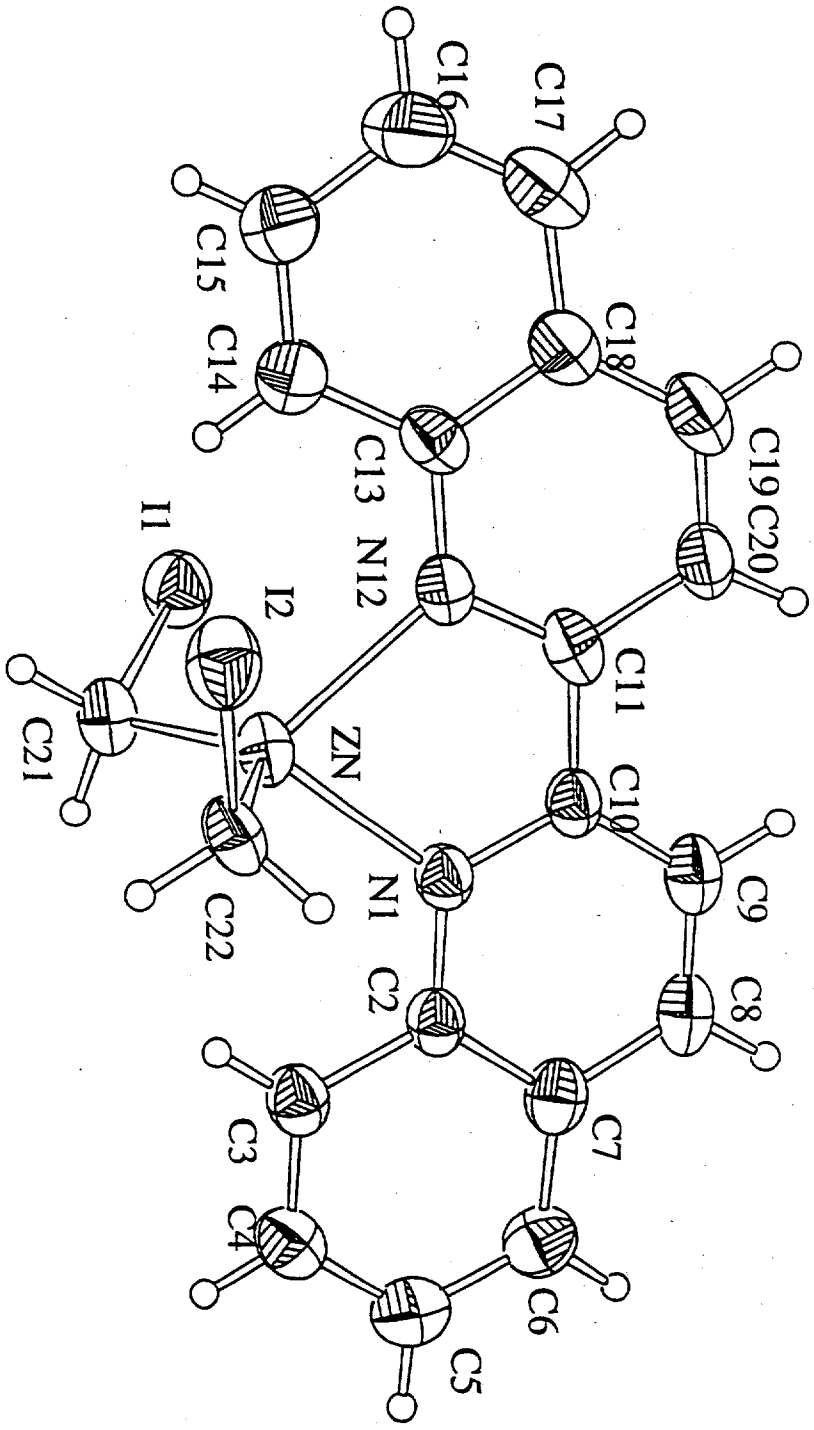
	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn	0.0640 (6)	0.0562 (5)	0.0437 (5)	0.0059 (4)	−0.0092 (4)	−0.0262 (4)
I1	0.0659 (4)	0.0836 (3)	0.0648 (3)	0.0115 (2)	−0.0136 (2)	−0.0351 (3)
I2	0.0919 (5)	0.0622 (3)	0.0563 (3)	0.0094 (3)	−0.0108 (3)	−0.0225 (2)
I3	0.091 (5)	0.106 (5)	0.058 (3)	0.030 (4)	−0.027 (3)	−0.041 (3)
N1	0.046 (3)	0.059 (3)	0.044 (3)	0.008 (2)	−0.010 (2)	−0.026 (2)
C2	0.046 (4)	0.055 (3)	0.041 (3)	0.011 (3)	−0.012 (3)	−0.023 (3)
C3	0.056 (4)	0.063 (4)	0.052 (4)	0.010 (3)	−0.014 (3)	−0.029 (3)
C4	0.062 (5)	0.070 (4)	0.070 (5)	0.007 (3)	−0.018 (4)	−0.037 (4)
C5	0.064 (5)	0.067 (4)	0.075 (5)	−0.002 (4)	−0.004 (4)	−0.029 (4)
C6	0.064 (5)	0.058 (4)	0.061 (4)	0.002 (3)	−0.005 (4)	−0.019 (3)
C7	0.062 (5)	0.059 (3)	0.050 (4)	0.014 (3)	−0.007 (3)	−0.025 (3)
C8	0.076 (5)	0.070 (4)	0.041 (3)	0.015 (4)	−0.007 (3)	−0.027 (3)
C9	0.073 (5)	0.073 (4)	0.042 (3)	0.011 (4)	−0.011 (3)	−0.030 (3)
C10	0.047 (4)	0.060 (3)	0.042 (3)	0.011 (3)	−0.010 (3)	−0.026 (3)
C11	0.058 (4)	0.061 (3)	0.057 (4)	0.019 (3)	−0.022 (3)	−0.038 (3)
N12	0.053 (3)	0.061 (3)	0.045 (3)	0.010 (2)	−0.010 (2)	−0.029 (2)
C13	0.052 (4)	0.056 (3)	0.065 (4)	0.008 (3)	−0.015 (3)	−0.039 (3)
C14	0.081 (6)	0.068 (4)	0.063 (5)	−0.010 (4)	0.003 (4)	−0.032 (4)
C15	0.076 (6)	0.077 (5)	0.078 (6)	−0.006 (4)	0.001 (5)	−0.038 (4)
C16	0.081 (7)	0.083 (5)	0.102 (7)	−0.015 (5)	−0.002 (6)	−0.046 (5)
C17	0.082 (7)	0.088 (6)	0.101 (7)	0.001 (5)	−0.028 (6)	−0.059 (6)
C18	0.054 (4)	0.068 (4)	0.072 (5)	0.012 (3)	−0.015 (4)	−0.042 (4)
C19	0.069 (5)	0.089 (5)	0.074 (5)	0.015 (4)	−0.026 (4)	−0.057 (5)
C20	0.060 (5)	0.081 (4)	0.051 (4)	0.010 (4)	−0.010 (3)	−0.041 (4)
C21	0.078 (6)	0.080 (5)	0.049 (4)	−0.003 (4)	−0.004 (4)	−0.036 (4)
C22	0.065 (6)	0.073 (5)	0.054 (5)	0.011 (4)	−0.026 (4)	−0.037 (4)

Table S3. *Geometric parameters (Å, °)*

Zn—I1	3.477 (4)	C9—C10	1.412 (10)
Zn—I2	3.551 (7)	C9—H9	0.9300
Zn—I3	2.514 (8)	C10—C11	1.464 (10)
Zn—C21	2.015 (8)	C11—N12	1.324 (9)
Zn—C22	2.082 (9)	C11—C20	1.415 (9)
Zn—N1	2.135 (7)	N12—C13	1.367 (9)
Zn—N12	2.141 (6)	C13—C14	1.403 (11)
I1—C21	2.142 (9)	C13—C18	1.410 (10)
I2—C22	2.106 (11)	C14—C15	1.357 (12)
N1—C10	1.355 (8)	C14—H14	0.9300
N1—C2	1.369 (9)	C15—C16	1.396 (13)
C2—C7	1.418 (10)	C15—H15	0.9300
C2—C3	1.433 (9)	C16—C17	1.319 (14)
C3—C4	1.364 (11)	C16—H16	0.9300
C3—H3	0.9300	C17—C18	1.444 (12)
C4—C5	1.393 (11)	C17—H17	0.9300
C4—H4	0.9300	C18—C19	1.393 (12)
C5—C6	1.356 (11)	C19—C20	1.368 (12)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.399 (11)	C20—H20	0.9300
C6—H6	0.9300	C21—H21A	0.9700
C7—C8	1.422 (10)	C21—H21B	0.9700
C8—C9	1.333 (11)	C22—H22A	0.9700
C8—H8	0.9300	C22—H22B	0.9700

C21—Zn—C22	125.5 (3)	C20—C11—C10	120.2 (7)
C21—Zn—N1	111.2 (3)	C11—N12—C13	120.5 (6)
C22—Zn—N1	105.6 (4)	C11—N12—Zn	114.9 (5)
C21—Zn—N12	113.1 (3)	C13—N12—Zn	124.5 (5)
C22—Zn—N12	113.5 (3)	N12—C13—C14	119.9 (6)
N1—Zn—N12	76.8 (2)	N12—C13—C18	120.2 (7)
C21—Zn—I3	125.4 (3)	C14—C13—C18	119.9 (7)
N1—Zn—I3	118.0 (3)	C15—C14—C13	120.1 (8)
N12—Zn—I3	100.2 (3)	C15—C14—H14	119.9
C10—N1—C2	119.4 (6)	C13—C14—H14	119.9
C10—N1—Zn	115.2 (5)	C14—C15—C16	120.8 (9)
C2—N1—Zn	125.4 (4)	C14—C15—H15	119.6
N1—C2—C7	122.3 (6)	C16—C15—H15	119.6
N1—C2—C3	118.4 (6)	C17—C16—C15	120.8 (9)
C7—C2—C3	119.3 (7)	C17—C16—H16	119.6
C4—C3—C2	118.5 (7)	C15—C16—H16	119.6
C4—C3—H3	120.8	C16—C17—C18	121.5 (9)
C2—C3—H3	120.8	C16—C17—H17	119.3
C3—C4—C5	121.7 (8)	C18—C17—H17	119.3
C3—C4—H4	119.1	C19—C18—C13	117.8 (7)
C5—C4—H4	119.1	C19—C18—C17	125.3 (8)
C6—C5—C4	120.8 (8)	C13—C18—C17	116.9 (8)
C6—C5—H5	119.6	C20—C19—C18	121.9 (7)
C4—C5—H5	119.6	C20—C19—H19	119.1
C5—C6—C7	120.4 (7)	C18—C19—H19	119.1
C5—C6—H6	119.8	C19—C20—C11	117.1 (7)
C7—C6—H6	119.8	C19—C20—H20	121.4
C6—C7—C2	119.3 (7)	C11—C20—H20	121.4
C6—C7—C8	124.1 (7)	Zn—C21—I1	113.5 (3)
C2—C7—C8	116.6 (7)	Zn—C21—H21A	108.9
C9—C8—C7	120.1 (7)	I1—C21—H21A	108.9
C9—C8—H8	119.9	Zn—C21—H21B	108.9
C7—C8—H8	119.9	I1—C21—H21B	108.9
C8—C9—C10	121.8 (7)	H21A—C21—H21B	107.7
C8—C9—H9	119.1	Zn—C22—I2	116.0 (5)
C10—C9—H9	119.1	Zn—C22—H22A	108.3
N1—C10—C9	119.8 (7)	I2—C22—H22A	108.3
N1—C10—C11	115.3 (6)	Zn—C22—H22B	108.3
C9—C10—C11	124.9 (6)	I2—C22—H22B	108.3
N12—C11—C20	122.3 (7)	H22A—C22—H22B	107.4
N12—C11—C10	117.5 (6)		

C21—Zn—N1—C10	112.9 (5)	C20—C11—N12—Zn	−173.4 (5)
C22—Zn—N1—C10	−108.2 (5)	C10—C11—N12—Zn	6.4 (7)
N12—Zn—N1—C10	3.0 (4)	C21—Zn—N12—C11	−112.7 (5)
I3—Zn—N1—C10	−91.7 (5)	C22—Zn—N12—C11	96.4 (6)
C21—Zn—N1—C2	−68.9 (6)	N1—Zn—N12—C11	−5.0 (4)
C22—Zn—N1—C2	70.0 (6)	I3—Zn—N12—C11	111.6 (5)
N12—Zn—N1—C2	−178.8 (5)	C21—Zn—N12—C13	71.2 (6)
I3—Zn—N1—C2	86.5 (6)	C22—Zn—N12—C13	−79.7 (6)
C10—N1—C2—C7	−1.5 (9)	N1—Zn—N12—C13	178.9 (6)
Zn—N1—C2—C7	−179.7 (5)	I3—Zn—N12—C13	−64.5 (6)
C10—N1—C2—C3	179.3 (6)	C11—N12—C13—C14	174.5 (7)
Zn—N1—C2—C3	1.2 (8)	Zn—N12—C13—C14	−9.6 (9)
N1—C2—C3—C4	−179.9 (6)	C11—N12—C13—C18	−3.7 (10)
C7—C2—C3—C4	1.0 (10)	Zn—N12—C13—C18	172.1 (5)
C2—C3—C4—C5	0.2 (11)	N12—C13—C14—C15	179.9 (8)
C3—C4—C5—C6	−1.1 (13)	C18—C13—C14—C15	−1.8 (12)
C4—C5—C6—C7	0.7 (12)	C13—C14—C15—C16	0.6 (14)
C5—C6—C7—C2	0.4 (11)	C14—C15—C16—C17	−1.0 (16)
C5—C6—C7—C8	179.4 (7)	C15—C16—C17—C18	2.6 (16)
N1—C2—C7—C6	179.6 (6)	N12—C13—C18—C19	1.2 (10)
C3—C2—C7—C6	−1.3 (10)	C14—C13—C18—C19	−177.1 (7)
N1—C2—C7—C8	0.5 (10)	N12—C13—C18—C17	−178.5 (7)
C3—C2—C7—C8	179.7 (6)	C14—C13—C18—C17	3.3 (11)
C6—C7—C8—C9	−178.9 (7)	C16—C17—C18—C19	176.6 (9)
C2—C7—C8—C9	0.1 (11)	C16—C17—C18—C13	−3.7 (14)
C7—C8—C9—C10	0.3 (12)	C13—C18—C19—C20	2.3 (12)
C2—N1—C10—C9	1.9 (9)	C17—C18—C19—C20	−178.0 (8)
Zn—N1—C10—C9	−179.8 (5)	C18—C19—C20—C11	−3.2 (12)
C2—N1—C10—C11	−179.0 (5)	N12—C11—C20—C19	0.6 (11)
Zn—N1—C10—C11	−0.7 (7)	C10—C11—C20—C19	−179.1 (7)
C8—C9—C10—N1	−1.3 (11)	C22—Zn—C21—I1	165.6 (4)
C8—C9—C10—C11	179.7 (7)	N1—Zn—C21—I1	−65.4 (4)
N1—C10—C11—N12	−3.8 (9)	N12—Zn—C21—I1	18.8 (5)
C9—C10—C11—N12	175.2 (6)	I3—Zn—C21—I1	141.4 (4)
N1—C10—C11—C20	176.0 (6)	C21—Zn—C22—I2	−98.3 (5)
C9—C10—C11—C20	−5.0 (10)	N1—Zn—C22—I2	130.4 (4)
C20—C11—N12—C13	2.8 (10)	N12—Zn—C22—I2	48.3 (5)
C10—C11—N12—C13	−177.4 (6)	I3—Zn—C22—I2	−1.5 (6)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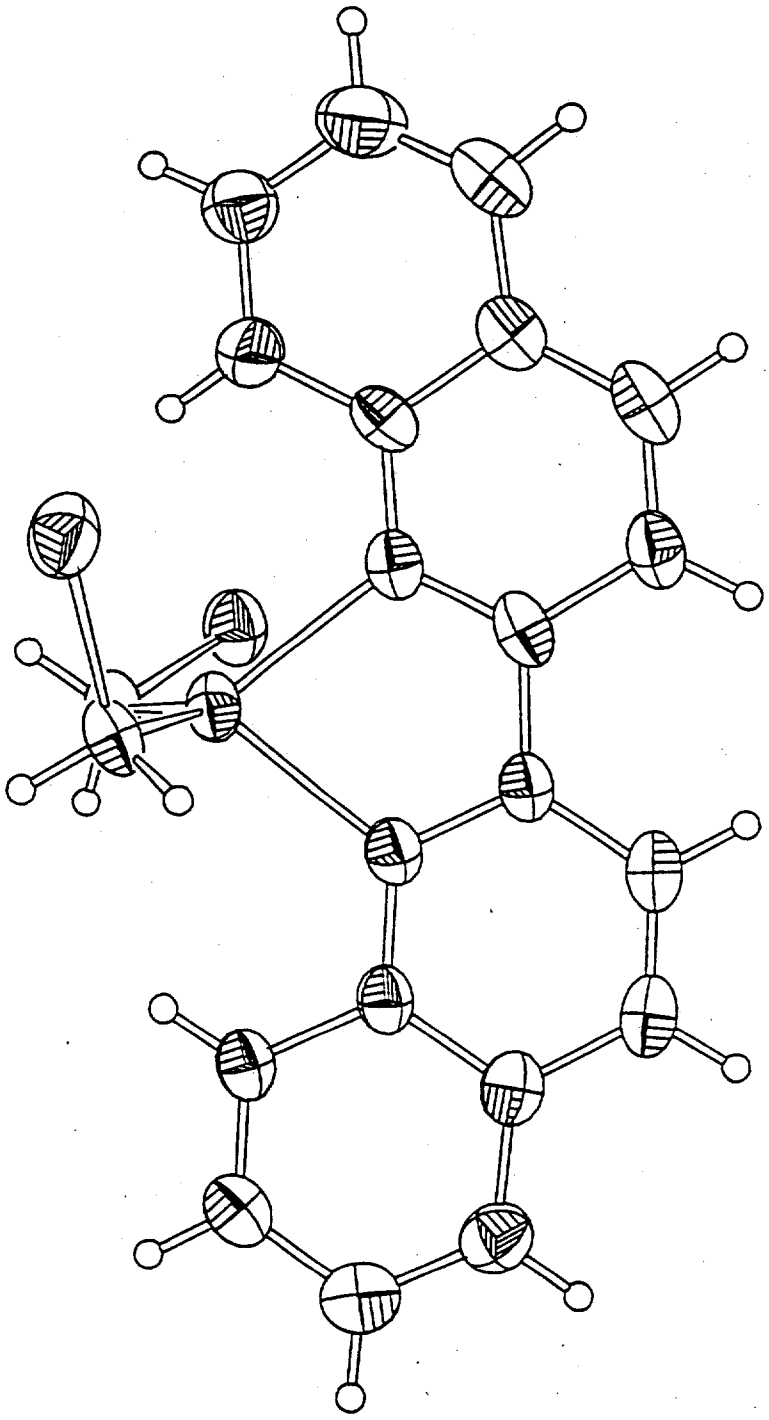
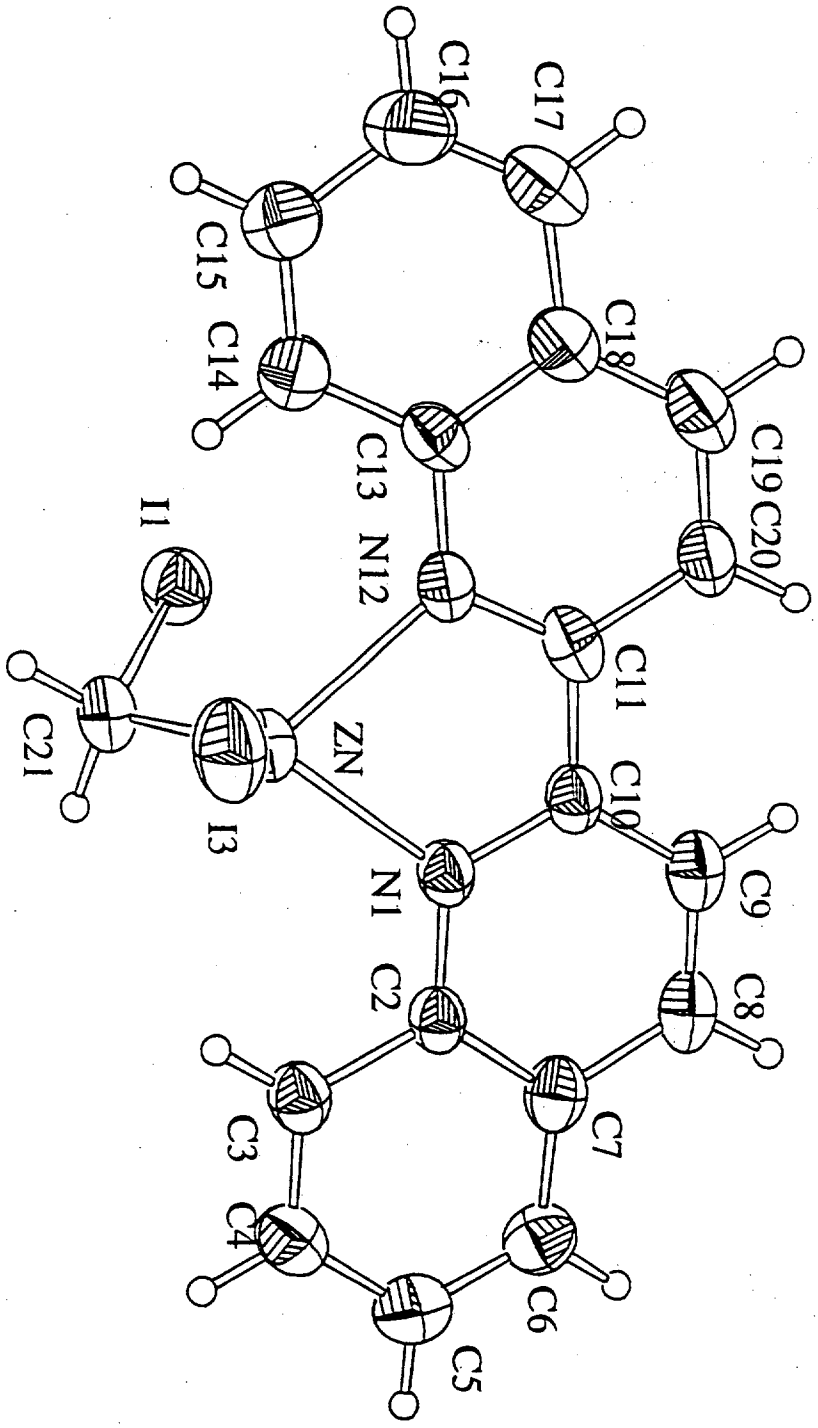
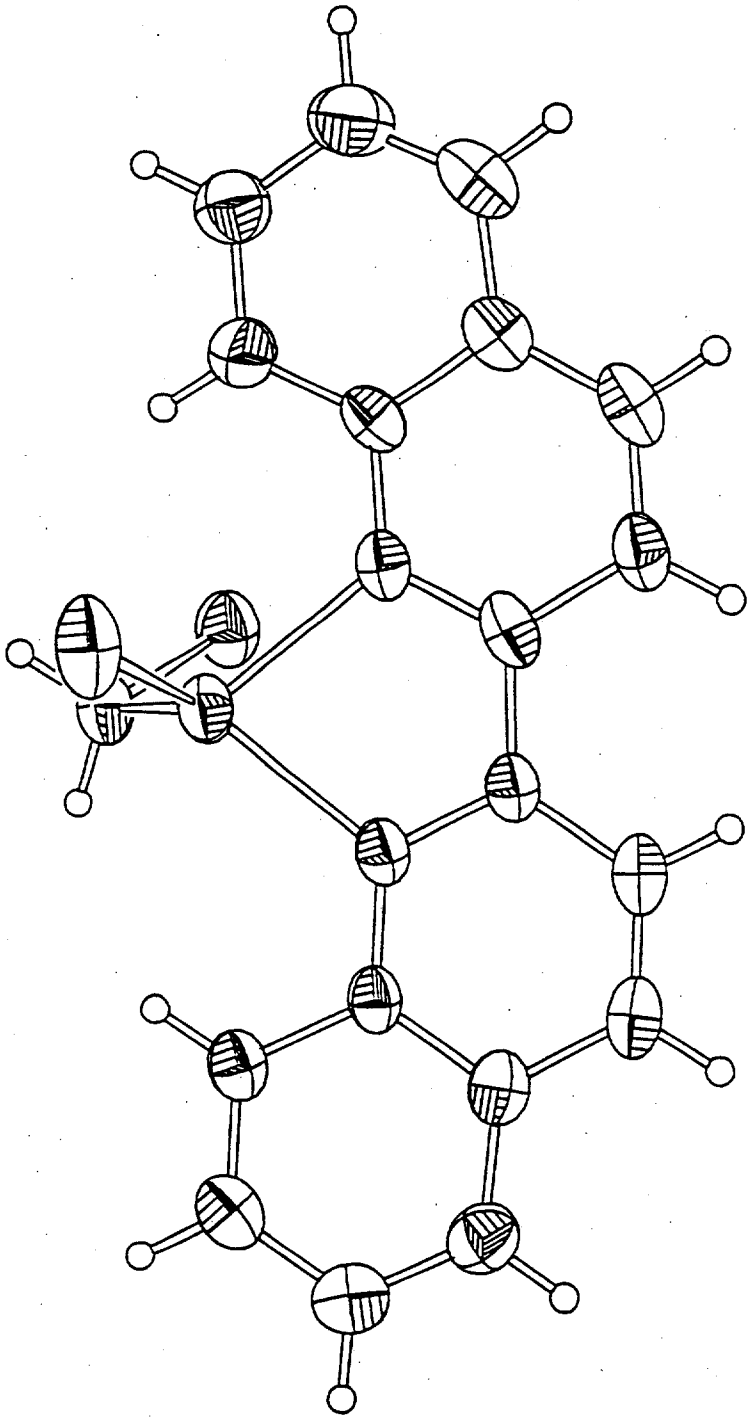
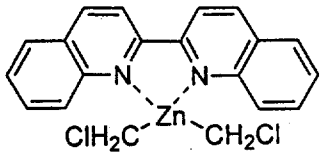






Crystal Data



Crystal data

$C_{20}H_{16}Cl_2N_2Zn$

$M_r = 420.628$

Monoclinic

$P2_1/n$

$a = 9.794(8)$ Å

$b = 18.747(11)$ Å

$c = 10.214(5)$ Å

$\beta = 101.36(5)°$

$V = 1839(2)$ Å^3

$Z = 4$

$D_x = 1.5195$ Mg m^{-3}

D_m not measured

Cu $K\alpha$ radiation

$\lambda = 1.54056$ Å

Cell parameters from 25 reflections

$\theta = 20.00–25.00°$

$\mu = 4.643$ mm^{-1}

$T = 293(2)$ K

Block

Clear red

0.57 × 0.24 × 0.10 mm

Crystal source: synthesized by the authors, see text

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scan
Absorption correction:
by integration ABSORP in *NRCVAX*
(Gabe *et al.* 1989)
$T_{min} = 0.2103, T_{max} = 0.6500$
21150 measured reflections
3484 independent reflections
2249 reflections with
$>2\sigma(I)$

$R_{int} = 0.089$
$\theta_{max} = 69.82°$
$h = -11 \rightarrow 11$
$k = -22 \rightarrow 22$
$l = -12 \rightarrow 12$
5 standard reflections
frequency: 60 min
intensity decay: 17.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.0604$
$wR(F^2) = 0.1751$
$S = 1.142$
3484 reflections
233 parameters
H-atom parameters constrained

$w=1/[\sigma^2(F_o^2) + (0.1229P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.520$ e Å^{-3}
$\Delta\rho_{min} = -0.751$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

Zn—Cl1	3.222 (2)	C5—C6	1.311 (8)
Zn—Cl2	3.168 (2)	C6—C7	1.417 (7)
Zn—Cl3	3.049 (9)	C7—C8	1.386 (7)
Zn—C23	1.986 (16)	C8—C9	1.359 (7)
Zn—C21	2.013 (5)	C9—C10	1.430 (6)
Zn—C22	2.054 (6)	C10—C11	1.504 (6)
Zn—N1	2.117 (4)	C11—N12	1.320 (5)
Zn—N12	2.137 (4)	C11—C20	1.411 (6)
Cl1—C21	1.787 (5)	N12—C13	1.374 (6)
Cl2—C22	1.690 (6)	C13—C14	1.405 (6)
Cl3—C23	1.668 (16)	C13—C18	1.422 (6)
N1—C10	1.293 (6)	C14—C15	1.361 (7)
N1—C2	1.383 (6)	C15—C16	1.368 (7)
C2—C7	1.407 (7)	C16—C17	1.379 (7)
C2—C3	1.418 (7)	C17—C18	1.417 (7)
C3—C4	1.382 (8)	C18—C19	1.386 (6)
C4—C5	1.376 (9)	C19—C20	1.359 (7)

C23—Zn—C21	115.7 (10)	N1—C10—C9	122.9 (4)
C21—Zn—C22	127.7 (3)	N1—C10—C11	117.0 (4)
C23—Zn—N1	131.1 (7)	C9—C10—C11	120.1 (4)
C21—Zn—N1	109.32 (17)	N12—C11—C20	122.4 (4)
C22—Zn—N1	109.2 (2)	N12—C11—C10	114.9 (4)
C23—Zn—N12	106.2 (12)	C20—C11—C10	122.7 (4)
C21—Zn—N12	111.92 (19)	C11—N12—C13	118.9 (4)
C22—Zn—N12	110.2 (3)	C11—N12—Zn	115.2 (3)
N1—Zn—N12	77.02 (15)	C13—N12—Zn	126.0 (3)
C10—N1—C2	119.2 (4)	N12—C13—C14	119.6 (4)
C10—N1—Zn	115.5 (3)	N12—C13—C18	121.2 (4)
C2—N1—Zn	125.1 (3)	C14—C13—C18	119.2 (4)
N1—C2—C7	121.1 (5)	C15—C14—C13	120.2 (5)
N1—C2—C3	118.5 (5)	C14—C15—C16	121.4 (5)
C7—C2—C3	120.4 (5)	C15—C16—C17	121.0 (5)
C4—C3—C2	118.5 (6)	C16—C17—C18	119.5 (5)
C5—C4—C3	119.8 (7)	C19—C18—C17	123.3 (5)
C6—C5—C4	122.7 (6)	C19—C18—C13	118.0 (4)
C5—C6—C7	121.2 (6)	C17—C18—C13	118.7 (4)
C8—C7—C2	117.9 (5)	C20—C19—C18	120.3 (4)
C8—C7—C6	124.8 (5)	C19—C20—C11	119.2 (4)
C2—C7—C6	117.3 (5)	Cl1—C21—Zn	115.8 (3)
C9—C8—C7	121.0 (5)	Cl2—C22—Zn	115.3 (4)
C8—C9—C10	117.9 (5)	Cl3—C23—Zn	112.8 (11)
C23—Zn—N1—C10	−105.8 (16)	C3—C4—C5—C6	0.7 (10)
C21—Zn—N1—C10	103.5 (3)	C4—C5—C6—C7	−0.4 (9)
C22—Zn—N1—C10	−112.6 (4)	N1—C2—C7—C8	−0.9 (7)
N12—Zn—N1—C10	−5.5 (3)	C3—C2—C7—C8	179.3 (4)
C23—Zn—N1—C2	79.4 (16)	N1—C2—C7—C6	178.8 (4)
C21—Zn—N1—C2	−71.3 (4)	C3—C2—C7—C6	−1.0 (7)
C22—Zn—N1—C2	72.6 (4)	C5—C6—C7—C8	−179.8 (5)
N12—Zn—N1—C2	179.7 (4)	C5—C6—C7—C2	0.6 (7)
C10—N1—C2—C7	−0.3 (6)	C2—C7—C8—C9	1.3 (7)
Zn—N1—C2—C7	174.3 (3)	C6—C7—C8—C9	−178.3 (4)
C10—N1—C2—C3	179.5 (4)	C7—C8—C9—C10	−0.6 (7)
Zn—N1—C2—C3	−5.9 (6)	C2—N1—C10—C9	1.2 (6)
N1—C2—C3—C4	−178.5 (5)	Zn—N1—C10—C9	−174.0 (3)
C7—C2—C3—C4	1.2 (8)	C2—N1—C10—C11	−177.2 (4)
C2—C3—C4—C5	−1.0 (9)	Zn—N1—C10—C11	7.7 (5)

C8—C9—C10—C11	177.5 (4)	C15—C16—C17—C18	−0.2 (7)
N1—C10—C11—N12	−5.8 (5)	C16—C17—C18—C19	179.3 (4)
C9—C10—C11—N12	175.9 (4)	C16—C17—C18—C13	−0.1 (6)
N1—C10—C11—C20	173.1 (4)	N12—C13—C18—C19	−0.2 (6)
C9—C10—C11—C20	−5.3 (6)	C14—C13—C18—C19	−179.4 (4)
C20—C11—N12—C13	0.9 (6)	N12—C13—C18—C17	179.3 (4)
C10—C11—N12—C13	179.7 (3)	C14—C13—C18—C17	0.1 (6)
C20—C11—N12—Zn	−178.0 (3)	C17—C18—C19—C20	−179.1 (4)
C10—C11—N12—Zn	0.8 (4)	C13—C18—C19—C20	0.3 (6)
C23—Zn—N12—C11	131.7 (7)	C18—C19—C20—C11	0.1 (7)
C21—Zn—N12—C11	−103.6 (3)	N12—C11—C20—C19	−0.7 (6)
C22—Zn—N12—C11	108.2 (3)	C10—C11—C20—C19	−179.5 (4)
N1—Zn—N12—C11	2.3 (3)	C23—Zn—C21—Cl1	−172.2 (10)
C23—Zn—N12—C13	−47.1 (7)	C22—Zn—C21—Cl1	−151.2 (3)
C21—Zn—N12—C13	77.6 (3)	N1—Zn—C21—Cl1	−15.9 (4)
C22—Zn—N12—C13	−70.6 (4)	N12—Zn—C21—Cl1	67.5 (3)
N1—Zn—N12—C13	−176.6 (3)	C23—Zn—C22—Cl2	5 (3)
C11—N12—C13—C14	178.8 (4)	C21—Zn—C22—Cl2	−53.1 (6)
Zn—N12—C13—C14	−2.4 (5)	N1—Zn—C22—Cl2	171.5 (4)
C11—N12—C13—C18	−0.4 (6)	N12—Zn—C22—Cl2	88.7 (5)
Zn—N12—C13—C18	178.3 (3)	C21—Zn—C23—Cl3	131.1 (18)
N12—C13—C14—C15	−178.9 (4)	C22—Zn—C23—Cl3	−1.7 (13)
C18—C13—C14—C15	0.4 (7)	N1—Zn—C23—Cl3	−19 (3)
C13—C14—C15—C16	−0.7 (8)	N12—Zn—C23—Cl3	−105 (2)

Data collection: CAD-4 software (Enraf–Nonius, 1989). Cell refinement: CAD-4 software (Enraf–Nonius, 1989). Data reduction: NRC-2, NRC-2A (Ahmed *et al.* 1973). Program(s) used to solve structure: *SHELXS*96 (Sheldrick, 1990). Program(s) used to refine structure: *NRCVAX* (Gabe *et al.* 1989) and *SHELXL*96 (Sheldrick, 1996). Molecular graphics: *ORTEP*II (Johnson (1976) in *NRCVAX* (Gabe *et al.*(1989)). Software used to prepare material for publication: *NRCVAX* (Gabe *et al.*(1989) and *SHELXL*96 (Sheldrick (1996)).

References

Ahmed, F. R., Hall, S. R., Pippy, M. E. & Huber, C. P. (1973). NRC Crystallographic Computer Programs for the IBM/360. Accession Nos. 133–147 in *J. Appl. Cryst.* 6, 309–346.

Enraf–Nonius (1989). CAD-4 Software. Version 5.0. Enraf–Nonius, Delft, The Netherlands.

Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* 22, 384–387.

International Tables for Crystallography (1992). Vol. C. Tables 4.2.6.8 and 6.1.1. 4, Dordrecht: Kluwer Academic Publishers.

Johnson, C. K. (1976). *ORTEP*II - A Fortran Thermal Ellipsoid Plot Program, Technical Report ORNL-5138. Oak Ridge National Laboratory, Tenessee, USA.

Sheldrick, G. M. (1990). *SHELXS*96. Program for the Solution *of Crystal Structures.* University of Göttingen, Germany.

Sheldrick, G. M. (1996). *SHELXL*96. Program for the Refinement *of Crystal Structures.* University of Göttingen, Germany.

Spek, A. L. (1995). *PLATON* Molecular Geometry Program, July 1995 version. University of Utrecht, Utrecht, Holland.

Fig. 1 *ORTEP* (Johnson, 1976) drawing of the molecule. Ellipsoids correspond to 40% probability.

Space group confirmed by *PLATON* program (Spek, 1995). Data reduction performed using a locally modified version of the NRC-2 program (Ahmed *et al.* 1973). The structure was solved by direct method using *SHELXS*96 (Sheldrick, 1990) and difmap synthesis using *NRCVAX* (Gabe *et al.*(1989) and *SHELXL*96 (Sheldrick, 1996). All non-H atoms anisotropic, H atoms isotropic. H atoms constrained to the parent site using a riding model; *SHELXL*96 defaults, C—H 0.93 to 0.97 Å. The isotropic factors, U_{iso} , were adjusted to 20% higher value of the parent site. A final verification of possible voids was performed using the VOID routine of the *PLATON* program (Spek, 1995).

Data collection: CAD-4 software (Enraf–Nonius, 1989). Cell refinement: CAD-4 software (Enraf–Nonius, 1989). Data reduction: NRC-2, NRC-2A (Ahmed *et al.* 1973). Program(s) used to solve structure: *SHELXS*96 (Sheldrick, 1990). Program(s) used to refine structure: *NRCVAX* (Gabe *et al.* 1989) and *SHELXL*96 (Sheldrick, 1996). Molecular graphics: *ORTEP*II (Johnson (1976) in *NRCVAX* (Gabe *et al.*(1989)). Software used to prepare material for publication: *NRCVAX* (Gabe *et al.*(1989) and *SHELXL*96 (Sheldrick (1996)).

Table S1. *Fractional atomic coordinates and equivalent isotropic displacement parameters ($Å^2$)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U^{ij} a^i a^j \mathbf{a}_i.\mathbf{a}_j.$$

	Occupancy	*x*	*y*	*z*	U_{eq}
Zn	1	0.22813 (7)	0.09505 (3)	0.85934 (7)	0.0725 (3)
Cl1	1	0.08458 (15)	0.10111 (7)	1.11717 (16)	0.0919 (4)
Cl2	0.811 (3)	0.4136 (2)	−0.01265 (10)	0.7308 (3)	0.1177 (7)
Cl3	0.189 (3)	0.2590 (10)	0.0235 (5)	0.5987 (11)	0.1177 (7)
N1	1	0.0712 (4)	0.1718 (2)	0.7926 (3)	0.0650 (9)
C2	1	−0.0674 (5)	0.1564 (3)	0.7426 (4)	0.0720 (12)
C3	1	−0.1077 (6)	0.0840 (3)	0.7225 (6)	0.0878 (15)
H3	1	−0.0428	0.0475	0.7444	0.105
C4	1	−0.2456 (7)	0.0687 (4)	0.6697 (6)	0.1011 (19)
H4	1	−0.2742	0.0216	0.6543	0.121
C5	1	−0.3405 (6)	0.1233 (4)	0.6399 (6)	0.1021 (19)
H5	1	−0.4330	0.1120	0.6053	0.123
C6	1	−0.3059 (6)	0.1907 (4)	0.6583 (5)	0.0893 (16)
H6	1	−0.3739	0.2256	0.6361	0.107
C7	1	−0.1668 (5)	0.2112 (3)	0.7115 (5)	0.0750 (13)
C8	1	−0.1217 (5)	0.2810 (3)	0.7345 (5)	0.0795 (14)
H8	1	−0.1858	0.3181	0.7165	0.095
C9	1	0.0146 (5)	0.2961 (3)	0.7828 (5)	0.0732 (12)
H9	1	0.0450	0.3429	0.7975	0.088
C10	1	0.1097 (5)	0.2376 (2)	0.8103 (4)	0.0624 (10)
C11	1	0.2626 (5)	0.2514 (2)	0.8587 (4)	0.0623 (10)
N12	1	0.3394 (4)	0.19366 (18)	0.8890 (3)	0.0593 (8)
C13	1	0.4804 (5)	0.2012 (2)	0.9335 (4)	0.0621 (10)
C14	1	0.5633 (5)	0.1404 (3)	0.9686 (5)	0.0738 (12)
H14	1	0.5228	0.0953	0.9602	0.089
C15	1	0.7029 (6)	0.1472 (3)	1.0150 (5)	0.0834 (14)
H15	1	0.7564	0.1065	1.0388	0.100
C16	1	0.7660 (6)	0.2126 (3)	1.0272 (5)	0.0846 (15)
H16	1	0.8617	0.2156	1.0583	0.102
C17	1	0.6900 (5)	0.2742 (3)	0.9942 (5)	0.0815 (14)
H17	1	0.7340	0.3184	1.0032	0.098
C18	1	0.5442 (5)	0.2696 (3)	0.9463 (4)	0.0654 (11)
C19	1	0.4597 (5)	0.3288 (3)	0.9121 (4)	0.0709 (12)
H19	1	0.4987	0.3742	0.9190	0.085
C20	1	0.3203 (5)	0.3207 (2)	0.8685 (4)	0.0692 (11)
H20	1	0.2635	0.3603	0.8454	0.083
C21	1	0.1988 (6)	0.0527 (3)	1.0328 (5)	0.0811 (14)
H21A	1	0.1622	0.0049	1.0154	0.097
H21B	1	0.2887	0.0487	1.0924	0.097
C22	0.811 (3)	0.2741 (8)	0.0422 (4)	0.6972 (7)	0.095 (2)
H22A	0.811 (3)	0.1934	0.0143	0.6565	0.113
H22B	0.811 (3)	0.2903	0.0773	0.6322	0.113
C23	0.189 (3)	0.335 (3)	0.0324 (18)	0.7590 (19)	0.095 (2)
H23A	0.189 (3)	0.4275	0.0522	0.7644	0.113
H23B	0.189 (3)	0.3450	−0.0143	0.8006	0.113

Table *S2. Anisotropic displacement parameters* ($Å^2$)

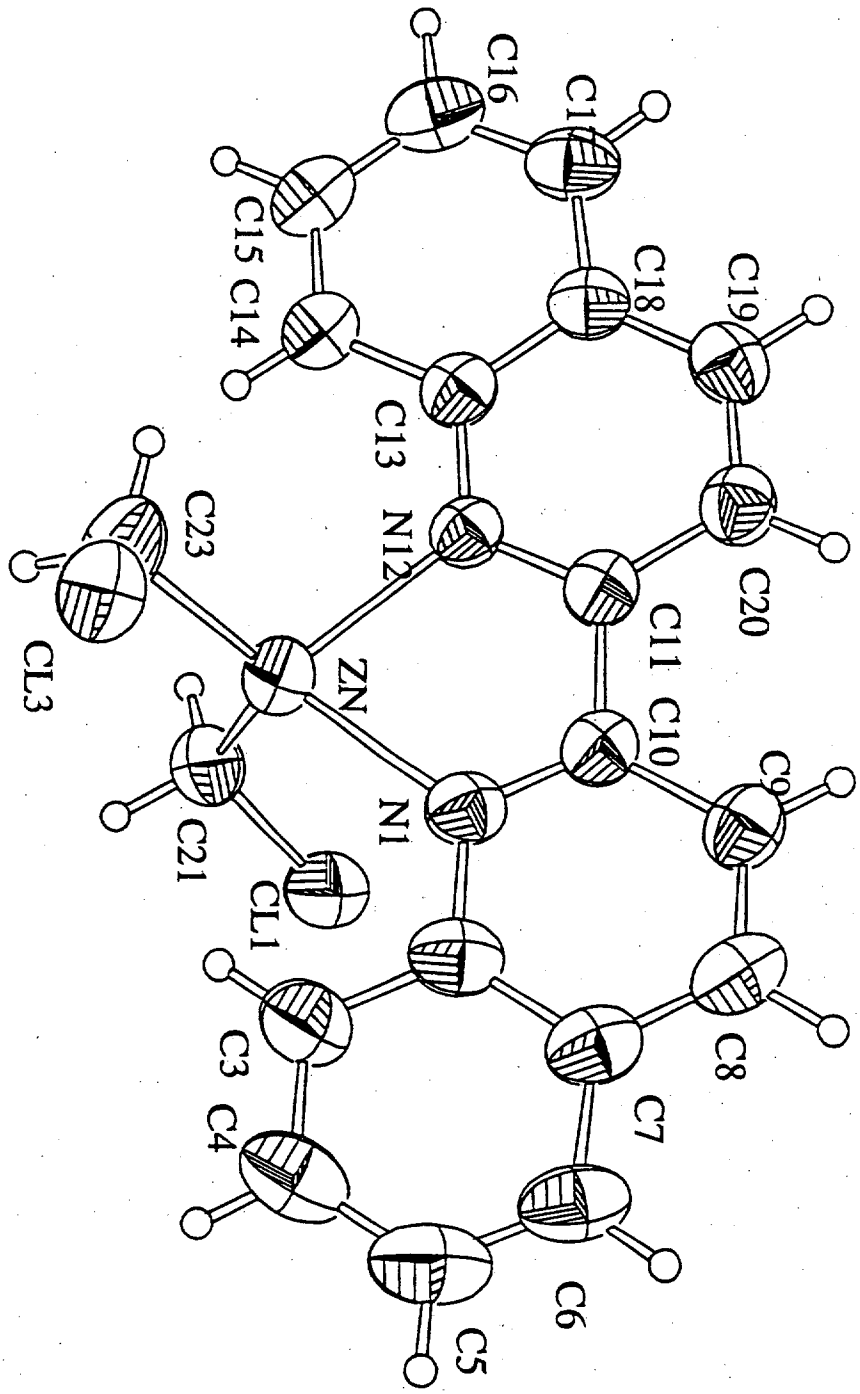
	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Zn	0.0725 (4)	0.0649 (4)	0.0816 (5)	0.0050 (3)	0.0188 (3)	−0.0004 (3)
Cl1	0.0775 (8)	0.0936 (9)	0.1079 (11)	−0.0048 (6)	0.0266 (7)	−0.0047 (7)
Cl2	0.1088 (15)	0.0871 (12)	0.163 (2)	0.0043 (10)	0.0401 (13)	−0.0215 (12)
Cl3	0.1088 (15)	0.0871 (12)	0.163 (2)	0.0043 (10)	0.0401 (13)	−0.0215 (12)
N1	0.061 (2)	0.072 (2)	0.063 (2)	0.0017 (17)	0.0144 (17)	0.0089 (17)
C2	0.067 (3)	0.094 (3)	0.057 (2)	−0.007 (2)	0.015 (2)	0.010 (2)
C3	0.080 (4)	0.091 (4)	0.090 (4)	−0.013 (3)	0.014 (3)	0.010 (3)
C4	0.097 (5)	0.119 (5)	0.087 (4)	−0.038 (4)	0.016 (3)	0.011 (3)
C5	0.069 (4)	0.151 (6)	0.084 (4)	−0.014 (4)	0.008 (3)	0.030 (4)
C6	0.062 (3)	0.135 (5)	0.072 (3)	0.002 (3)	0.019 (2)	0.017 (3)
C7	0.067 (3)	0.105 (4)	0.057 (3)	0.008 (3)	0.021 (2)	0.014 (2)
C8	0.065 (3)	0.103 (4)	0.072 (3)	0.021 (3)	0.018 (2)	0.012 (3)
C9	0.079 (3)	0.075 (3)	0.066 (3)	0.013 (2)	0.015 (2)	0.006 (2)
C10	0.065 (3)	0.070 (3)	0.054 (2)	0.007 (2)	0.018 (2)	0.0065 (19)
C11	0.069 (3)	0.066 (2)	0.054 (2)	0.005 (2)	0.018 (2)	0.0053 (19)
N12	0.060 (2)	0.0639 (19)	0.0555 (19)	0.0040 (16)	0.0149 (16)	0.0012 (15)
C13	0.068 (3)	0.070 (3)	0.051 (2)	0.005 (2)	0.019 (2)	−0.0019 (19)
C14	0.070 (3)	0.076 (3)	0.077 (3)	0.008 (2)	0.018 (2)	−0.002 (2)
C15	0.075 (3)	0.097 (4)	0.080 (3)	0.024 (3)	0.019 (3)	0.000 (3)
C16	0.065 (3)	0.121 (5)	0.069 (3)	0.005 (3)	0.016 (2)	−0.009 (3)
C17	0.072 (3)	0.109 (4)	0.067 (3)	−0.011 (3)	0.022 (2)	−0.011 (3)
C18	0.067 (3)	0.081 (3)	0.052 (2)	−0.002 (2)	0.019 (2)	−0.003 (2)
C19	0.086 (3)	0.068 (3)	0.061 (2)	−0.008 (2)	0.021 (2)	0.001 (2)
C20	0.077 (3)	0.065 (3)	0.067 (3)	0.006 (2)	0.018 (2)	0.004 (2)
C21	0.080 (3)	0.068 (3)	0.096 (4)	0.001 (2)	0.018 (3)	0.015 (3)
C22	0.110 (6)	0.098 (5)	0.068 (4)	0.027 (4)	−0.001 (4)	−0.026 (4)
C23	0.110 (6)	0.098 (5)	0.068 (4)	0.027 (4)	−0.001 (4)	−0.026 (4)

Table *S3. Geometric parameters* (*Å*, °)

Zn—Cl1	3.222 (2)	C9—C10	1.430 (6)
Zn—Cl2	3.168 (2)	C9—H9	0.9300
Zn—Cl3	3.049 (9)	C10—C11	1.504 (6)
Zn—C23	1.986 (16)	C11—N12	1.320 (5)
Zn—C21	2.013 (5)	C11—C20	1.411 (6)
Zn—C22	2.054 (6)	N12—C13	1.374 (6)
Zn—N1	2.117 (4)	C13—C14	1.405 (6)
Zn—N12	2.137 (4)	C13—C18	1.422 (6)
Cl1—C21	1.787 (5)	C14—C15	1.361 (7)
Cl2—C22	1.690 (6)	C14—H14	0.9300
Cl3—C23	1.668 (16)	C15—C16	1.368 (7)
N1—C10	1.293 (6)	C15—H15	0.9300
N1—C2	1.383 (6)	C16—C17	1.379 (7)
C2—C7	1.407 (7)	C16—H16	0.9300
C2—C3	1.418 (7)	C17—C18	1.417 (7)
C3—C4	1.382 (8)	C17—H17	0.9300
C3—H3	0.9300	C18—C19	1.386 (6)
C4—C5	1.376 (9)	C19—C20	1.359 (7)
C4—H4	0.9300	C19—H19	0.9300
C5—C6	1.311 (8)	C20—H20	0.9300
C5—H5	0.9300	C21—H21A	0.9700
C6—C7	1.417 (7)	C21—H21B	0.9700
C6—H6	0.9300	C22—H22A	0.9700
C7—C8	1.386 (7)	C22—H22B	0.9700
C8—C9	1.359 (7)	C23—H23A	0.9700
C8—H8	0.9300	C23—H23B	0.9700

C23—Zn—C21	113.7 (10)	C13—N12—Zn	126.0 (3)
C21—Zn—C22	127.7 (3)	N12—C13—C14	119.6 (4)
C23—Zn—N1	131.1 (7)	N12—C13—C18	121.2 (4)
C21—Zn—N1	109.32 (17)	C14—C13—C18	119.2 (4)
C22—Zn—N1	109.2 (2)	C15—C14—C13	120.2 (5)
C23—Zn—N12	106.2 (12)	C15—C14—H14	119.9
C21—Zn—N12	111.92 (19)	C13—C14—H14	119.9
C22—Zn—N12	110.2 (3)	C14—C15—C16	121.4 (5)
N1—Zn—N12	77.02 (15)	C14—C15—H15	119.3
C10—N1—C2	119.2 (4)	C16—C15—H15	119.3
C10—N1—Zn	115.5 (3)	C15—C16—C17	121.0 (5)
C2—N1—Zn	125.1 (3)	C15—C16—H16	119.5
N1—C2—C7	121.1 (5)	C17—C16—H16	119.5
N1—C2—C3	118.5 (5)	C16—C17—C18	119.5 (5)
C7—C2—C3	120.4 (5)	C16—C17—H17	120.3
C4—C3—C2	118.5 (6)	C18—C17—H17	120.3
C4—C3—H3	120.7	C19—C18—C17	123.3 (5)
C2—C3—H3	120.7	C19—C18—C13	118.0 (4)
C5—C4—C3	119.8 (7)	C17—C18—C13	118.7 (4)
C5—C4—H4	120.1	C20—C19—C18	120.3 (4)
C3—C4—H4	120.1	C20—C19—H19	119.9
C6—C5—C4	122.7 (6)	C18—C19—H19	119.9
C6—C5—H5	118.6	C19—C20—C11	119.2 (4)
C4—C5—H5	118.6	C19—C20—H20	120.4
C5—C6—C7	121.2 (6)	C11—C20—H20	120.4
C5—C6—H6	119.4	Cl1—C21—Zn	115.8 (3)
C7—C6—H6	119.4	Cl1—C21—H21A	108.3
C8—C7—C2	117.9 (5)	Zn—C21—H21A	108.3
C8—C7—C6	124.8 (5)	Cl1—C21—H21B	108.3
C2—C7—C6	117.3 (5)	Zn—C21—H21B	108.3
C9—C8—C7	121.0 (5)	H21A—C21—H21B	107.4
C9—C8—H8	119.5	Cl2—C22—Zn	115.3 (4)
C7—C8—H8	119.5	Cl2—C22—H22A	108.5
C8—C9—C10	117.9 (5)	Zn—C22—H22A	108.5
C8—C9—H9	121.1	Cl2—C22—H22B	108.5
C10—C9—H9	121.1	Zn—C22—H22B	108.5
N1—C10—C9	122.9 (4)	H22A—C22—H22B	107.5
N1—C10—C11	117.0 (4)	Cl3—C23—Zn	112.8 (11)
C9—C10—C11	120.1 (4)	Cl3—C23—H23A	109.0
N12—C11—C20	122.4 (4)	Zn—C23—H23A	109.0
N12—C11—C10	114.9 (4)	Cl3—C23—H23B	109.0
C20—C11—C10	122.7 (4)	Zn—C23—H23B	109.0
C11—N12—C13	118.9 (4)	H23A—C23—H23B	107.8
C11—N12—Zn	115.2 (3)		

C23—Zn—N1—C10	−105.8 (16)	C23—Zn—N12—C11	131.7 (7)
C21—Zn—N1—C10	103.5 (3)	C21—Zn—N12—C11	−103.6 (3)
C22—Zn—N1—C10	−112.6 (4)	C22—Zn—N12—C11	108.2 (3)
N12—Zn—N1—C10	−5.5 (3)	N1—Zn—N12—C11	2.3 (3)
C23—Zn—N1—C2	79.4 (16)	C23—Zn—N12—C13	−47.1 (7)
C21—Zn—N1—C2	−71.3 (4)	C21—Zn—N12—C13	77.6 (3)
C22—Zn—N1—C2	72.6 (4)	C22—Zn—N12—C13	−70.6 (4)
N12—Zn—N1—C2	179.7 (4)	N1—Zn—N12—C13	−176.6 (3)
C10—N1—C2—C7	−0.3 (6)	C11—N12—C13—C14	178.8 (4)
Zn—N1—C2—C7	174.3 (3)	Zn—N12—C13—C14	−2.4 (5)
C10—N1—C2—C3	179.5 (4)	C11—N12—C13—C18	−0.4 (6)
Zn—N1—C2—C3	−5.9 (6)	Zn—N12—C13—C18	178.3 (3)
N1—C2—C3—C4	−178.5 (5)	N12—C13—C14—C15	−178.9 (4)
C7—C2—C3—C4	1.2 (8)	C18—C13—C14—C15	0.4 (7)
C2—C3—C4—C5	−1.0 (9)	C13—C14—C15—C16	−0.7 (8)
C3—C4—C5—C6	0.7 (10)	C14—C15—C16—C17	0.7 (8)
C4—C5—C6—C7	−0.4 (9)	C15—C16—C17—C18	−0.2 (7)
N1—C2—C7—C8	−0.9 (7)	C16—C17—C18—C19	179.3 (4)
C3—C2—C7—C8	179.3 (4)	C16—C17—C18—C13	−0.1 (6)
N1—C2—C7—C6	178.8 (4)	N12—C13—C18—C19	−0.2 (6)
C3—C2—C7—C6	−1.0 (7)	C14—C13—C18—C19	−179.4 (4)
C5—C6—C7—C8	−179.8 (5)	N12—C13—C18—C17	179.3 (4)
C5—C6—C7—C2	0.6 (7)	C14—C13—C18—C17	0.1 (6)
C2—C7—C8—C9	1.3 (7)	C17—C18—C19—C20	−179.1 (4)
C6—C7—C8—C9	−178.3 (4)	C13—C18—C19—C20	0.3 (6)
C7—C8—C9—C10	−0.6 (7)	C18—C19—C20—C11	0.1 (7)
C2—N1—C10—C9	1.2 (6)	N12—C11—C20—C19	−0.7 (6)
Zn—N1—C10—C9	−174.0 (3)	C10—C11—C20—C19	−179.5 (4)
C2—N1—C10—C11	−177.2 (4)	C23—Zn—C21—Cl1	−172.2 (10)
Zn—N1—C10—C11	7.7 (5)	C22—Zn—C21—Cl1	−151.2 (3)
C8—C9—C10—N1	−0.7 (6)	N1—Zn—C21—Cl1	−15.9 (4)
C8—C9—C10—C11	177.5 (4)	N12—Zn—C21—Cl1	67.5 (3)
N1—C10—C11—N12	−5.8 (5)	C23—Zn—C22—Cl2	5 (3)
C9—C10—C11—N12	175.9 (4)	C21—Zn—C22—Cl2	−53.1 (6)
N1—C10—C11—C20	173.1 (4)	N1—Zn—C22—Cl2	171.5 (4)
C9—C10—C11—C20	−5.3 (6)	N12—Zn—C22—Cl2	88.7 (5)
C20—C11—N12—C13	0.9 (6)	C21—Zn—C23—Cl3	131.1 (18)
C10—C11—N12—C13	179.7 (3)	C22—Zn—C23—Cl3	−1.7 (13)
C20—C11—N12—Zn	−178.0 (3)	N1—Zn—C23—Cl3	−19 (3)
C10—C11—N12—Zn	0.8 (4)	N12—Zn—C23—Cl3	−105 (2)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