Inorganic Chemistry
including bioinorganic chemistry
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Table I. Experimental details of data collection and structure refinement in the X-ray crystallographic analysis of (CH=CH-*N*,*N*')[(OEP)Co^{II}Cl][(TPP)Zn^{II}Cl](**15b**)•CH_2Cl_2.

A. Crystal Data

Empirical Formula	$C_{82}H_{74}N_8CoZnCl_2$•CH_2Cl_2
Formula Weight	1451.7
Crystal Color, Habit	black, prismatic
Crystal Dimensions	0.15 X 0.40 X 0.40 mm
Crystal System	Triclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	20 (7.4 - 15.0°)
Omega Scan Peak Width at Half-height	0.49°
Lattice Parameters	a = 14.806(4) Å b = 18.703(10) Å c = 13.796(3) Å α = 97.69(3)° ß = 99.57(2)° γ = 96.74(3)° V = 3694(2) Å^3
Space Group	P-1 (#2)
Z value	2
D_{calc}	1.305 g/cm^3
F_{000}	1510
μ(MoKα)	7.44 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC5R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated
Attenuator	Zr foil (factors = 1.00, 1.11, 1.25, 1.39)
Detector Aperture	9.0 mm horizontal 13.0 mm vertical
Crystal to Detector Distance	258 mm
Temperature	24.0 °C
Scan Type	2θ–ω

Scan Rate	16.0 ° / min (in ω) (up to 3 scans)
Scan Width	(1.05 + 0.35 tan θ)
$2\theta_{max}$	50.0°
No. of Reflections Measured	Total: 13562 Unique: 13010 (R_{int} = 0.015)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.8259 - 1.0000) Decay (0.82 % increase)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SIR92)
Refinement	Full-matrix least-squares
Function Minimized	$\sum\omega(\|F_o\| - \|F_c\|)^2$ $\omega = 4F_o^2 / \sigma^2(F_o^2)$ $\sigma^2(F_o^2) = [S^2(C + R^2B) + (pF_o^2)^2] / Lp^2$ S = scan rate C = total integrated peak count R = ratio of scan time to background counting time B = total background count Lp = Lorentz-polarization factor p = p-factor
p-factor	0.0050
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I > 3.0\sigma(I)$)	8239
No. Variables	906
Reflection / Parameter Ratio	9.09
Residuals: $R = \sum(\|F_o\| - \|F_c\|) / \sum F_o$	0.059
$R_w = [\sum\omega(\|F_o\| - \|F_c\|)^2 / \sum\omega F_o^2]^{1/2}$	0.042
Goodness of Fit Indicator	2.72
Max Shift / Error in Final Cycle	0.01
Maximum peak in Final Diff. Map	0.99 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.68 $e^-/Å^3$

Table II. Positional parameters for (15b)·CH_2Cl_2.

atom	x	y	z	occupancy	B(eq)
Zn	.69351(4)	.39776(3)	.67906(5)	1.000	3.58(2)
Co	.77726(5)	.07424(4)	.47953(5)	1.000	3.32(2)
CL1	.7275(1)	-.03560(8)	.5207(1)	1.000	4.82(4)
CL2	.7418(1)	.50548(8)	.6380(1)	1.000	6.24(5)
N1	.7024(3)	.1418(2)	.5969(3)	1.000	2.9(1)
N2	.8931(3)	.1165(2)	.5859(3)	1.000	3.1(1)
N3	.8551(3)	.0771(2)	.3740(3)	1.000	3.7(1)
N4	.6654(3)	.0952(2)	.3827(3)	1.000	3.5(1)
N5	.7195(3)	.3282(2)	.5156(3)	1.000	3.0(1)
N6	.8169(3)	.3606(2)	.7325(3)	1.000	3.1(1)
N7	.6511(3)	.3854(2)	.8080(3)	1.000	3.4(1)
N8	.5568(3)	.3676(2)	.6021(3)	1.000	3.0(1)
C1	.6052(3)	.1212(3)	.5832(4)	1.000	2.9(1)
C2	.5813(4)	.1141(3)	.6761(4)	1.000	3.3(1)
C3	.6616(4)	.1259(3)	.7464(4)	1.000	3.8(2)
C4	.7385(4)	.1399(3)	.6984(4)	1.000	3.2(1)
C5	.8310(4)	.1471(3)	.7380(4)	1.000	3.8(1)
C6	.9043(4)	.1391(3)	.6856(4)	1.000	3.4(1)
C7	1.0001(4)	.1506(3)	.7339(4)	1.000	3.8(2)
C8	1.0490(4)	.1327(3)	.6615(4)	1.000	3.8(2)
C9	.9820(4)	.1115(3)	.5692(4)	1.000	3.4(1)
C10	1.0058(4)	.0901(3)	.4770(5)	1.000	4.0(2)
C11	.9471(4)	.0775(3)	.3851(4)	1.000	4.1(2)
C12	.9768(4)	.0701(4)	.2910(5)	1.000	5.9(2)
C13	.9004(5)	.0690(4)	.2209(5)	1.000	5.6(2)
C14	.8231(4)	.0735(3)	.2737(5)	1.000	4.4(2)
C15	.7320(4)	.0746(3)	.2316(4)	1.000	5.1(2)
C16	.6590(4)	.0853(3)	.2826(4)	1.000	4.3(2)
C17	.5645(4)	.0845(3)	.2327(5)	1.000	5.1(2)
C18	.5123(4)	.0938(3)	.3044(4)	1.000	4.2(2)
C19	.5765(4)	.1008(3)	.3983(4)	1.000	3.4(1)
C20	.5486(3)	.1076(3)	.4911(4)	1.000	3.2(1)
C21	.4844(4)	.0968(3)	.6930(4)	1.000	4.5(2)
C22	.4402(4)	.1644(4)	.7125(6)	1.000	9.6(3)
C23	.6707(4)	.1211(4)	.8555(5)	1.000	6.1(2)
C24	.6763(8)	.1929(6)	.9139(7)	.700	8.8(4)
C24'	.703(2)	.058(2)	.890(2)	.300	10.0(9)
C25	.0383(4)	.1785(3)	.8422(5)	1.000	5.5(2)
C26	1.0541(6)	.1199(4)	.9030(5)	1.000	9.5(3)
C27	1.1523(4)	.1397(3)	.6691(4)	1.000	5.2(2)
C28	1.1915(4)	.2086(4)	.6334(5)	1.000	7.3(2)
C29	1.070(1)	.0497(8)	.271(1)	.700	6.0(4)
C29'	1.083(2)	.098(2)	.281(2)	.300	4.2(8)

atom	x	y	z	occupancy	B(eq)
C30	1.125(1)	.114(1)	.266(2)	.700	10.6(6)
C30'	1.125(2)	.037(2)	.227(3)	.300	9.4(10)
C31	.8896(5)	.0665(4)	.1085(6)	1.000	8.1(3)
C32	.8900(5)	.1416(5)	.0869(6)	1.000	10.5(3)
C33	.5299(4)	.0693(4)	.1182(6)	1.000	7.2(2)
C34	.5310(8)	.1373(5)	.0822(6)	1.000	13.4(4)
C35	.4106(4)	.0974(4)	.2940(4)	1.000	5.5(2)
C36	.3895(4)	.1734(4)	.3289(5)	1.000	7.4(2)
C37	.7361(3)	.2110(3)	.5682(4)	1.000	3.1(1)
C38	.6846(3)	.2594(3)	.5429(4)	1.000	2.9(1)
C39	.6641(4)	.3546(3)	.4360(4)	1.000	3.3(1)
C40	.7271(4)	.3835(3)	.3804(4)	1.000	4.2(2)
C41	.8149(4)	.3786(3)	.4239(4)	1.000	4.1(2)
C42	.8137(3)	.3463(3)	.5100(4)	1.000	3.0(1)
C43	.8897(3)	.3429(3)	.5831(4)	1.000	3.2(1)
C44	.8896(3)	.3454(3)	.6839(4)	1.000	3.0(1)
C45	.9675(3)	.3375(3)	.7570(4)	1.000	3.8(1)
C46	.9437(4)	.3494(3)	.8467(4)	1.000	3.9(2)
C47	.8509(4)	.3648(3)	.8323(4)	1.000	3.3(1)
C48	.8022(4)	.3822(3)	.9103(4)	1.000	3.5(1)
C49	.7106(4)	.3921(3)	.8981(4)	1.000	3.7(2)
C50	.6582(4)	.4072(3)	.9763(4)	1.000	4.7(2)
C51	.5706(4)	.4076(3)	.9323(4)	1.000	4.7(2)
C52	.5645(4)	.3930(3)	.8269(4)	1.000	3.5(1)
C53	.4853(4)	.3841(3)	.7533(4)	1.000	3.4(1)
C54	.4817(3)	.3696(3)	.6518(4)	1.000	3.2(1)
C55	.3971(4)	.3552(3)	.5786(4)	1.000	4.1(2)
C56	.4205(4)	.3481(3)	.4885(4)	1.000	3.9(2)
C57	.5192(3)	.3575(3)	.5030(4)	1.000	3.2(1)
C58	.5703(3)	.3569(3)	.4252(4)	1.000	3.1(1)
C59	.9775(3)	.3438(3)	.5436(4)	1.000	3.5(1)
C60	.9860(4)	.2907(3)	.4676(4)	1.000	4.4(2)
C61	1.0639(5)	.2934(3)	.4238(5)	1.000	5.4(2)
C62	1.1343(4)	.3499(4)	.4558(5)	1.000	5.6(2)
C63	1.1280(4)	.4023(4)	.5309(6)	1.000	6.5(2)
C64	1.0504(4)	.3998(3)	.5761(5)	1.000	5.3(2)
C65	.8549(4)	.3900(3)	1.0143(4)	1.000	4.1(2)
C66	.8416(6)	.3387(4)	1.0734(5)	1.000	9.0(3)
C67	.8924(6)	.3461(4)	1.1703(6)	1.000	9.8(3)
C68	.9538(5)	.4065(4)	1.2087(5)	1.000	6.2(2)
C69	.9645(5)	.4590(4)	1.1526(6)	1.000	6.2(2)
C70	.9148(4)	.4510(3)	1.0575(5)	1.000	5.2(2)
C71	.3952(4)	.3912(3)	.7881(4)	1.000	3.8(2)

Table II. Continued.

atom	x	y	z	occupancy	B(eq)
C72	.3592(4)	.3412(3)	.8413(4)	1.000	4.9(2)
C73	.2757(5)	.3480(4)	.8736(5)	1.000	6.1(2)
C74	.2289(4)	.4051(4)	.8512(5)	1.000	6.3(2)
C75	.2643(4)	.4544(4)	.7990(5)	1.000	6.2(2)
C76	.3470(4)	.4477(3)	.7674(4)	1.000	5.3(2)
C77	.5232(3)	.3667(3)	.3250(4)	1.000	3.3(1)
C78	.5380(4)	.3246(3)	.2395(5)	1.000	4.5(2)
C79	.4949(5)	.3344(3)	.1464(4)	1.000	5.3(2)
C80	.4373(4)	.3861(4)	.1358(4)	1.000	5.2(2)
C81	.4213(4)	.4281(3)	.2193(5)	1.000	4.5(2)
C82	.4650(4)	.4192(3)	.3125(4)	1.000	3.8(2)
H5	.8477	.1587	.8085	1.000	4.5
H10	1.0685	.0837	.4772	1.000	4.8
H15	.7172	.0677	.1608	1.000	6.1
H20	.4838	.1020	.4900	1.000	3.8
H21A	.4485	.0661	.6358	1.000	5.4
H21B	.4858	.0718	.7489	1.000	5.4
H22A	.4377	.1892	.6571	1.000	11.4
H22B	.3790	.1509	.7237	1.000	11.4
H22C	.4754	.1951	.7701	1.000	11.4
H23A	.7254	.1006	.8767	.700	7.2
H23B	.6185	.0900	.8660	.700	7.2
H23C	.6119	.1243	.8731	.300	7.2
H23D	.7140	.1610	.8910	.300	7.2
H24A	.6875	.1885	.9811	.700	9.4
H24B	.6192	.2099	.8954	.700	9.4
H24C	.7249	.2235	.8971	.700	9.4
H24D	.6529	.0345	.9150	.300	9.6
H24E	.7105	.0273	.8309	.300	9.6
H24F	.7549	.0717	.9345	.300	9.6
H25A	.9955	.2066	.8680	1.000	6.6
H25B	1.0955	.2090	.8468	1.000	6.6
H26A	.9974	.0895	.8995	1.000	11.4
H26B	1.0973	.0920	.8786	1.000	11.4
H26C	1.0780	.1414	.9704	1.000	11.4
H27A	1.1667	.0984	.6296	1.000	6.2
H27B	1.1800	.1409	.7367	1.000	6.2
H28A	1.1775	.2500	.6727	1.000	8.7
H28B	1.2567	.2108	.6401	1.000	8.7
H28C	1.1648	.2074	.5658	1.000	8.7
H29A	1.0965	.0262	.3228	.700	6.9
H29B	1.0604	.0183	.2091	.700	6.9
H29C	1.0906	.1483	.2291	.300	14.1

atom	x	y	z	occupancy	B(eq)
H29D	1.1318	.1186	.3433	.300	7.4
H30A	1.1785	.1101	.2397	.700	14.1
H30B	1.1461	.1454	.3339	.700	14.1
H30C	1.0921	.1468	.2254	.700	4.0
H30D	1.1102	.0660	.1651	.300	10.1
H30E	1.1823	.0551	.2553	.300	10.1
H30F	1.1143	-.0111	.1939	.300	10.1
H31A	.9396	.0463	.0854	1.000	9.5
H31B	.8329	.0374	.0761	1.000	9.5
H32A	.8833	.1412	.0170	1.000	12.6
H32B	.9465	.1705	.1195	1.000	12.6
H32C	.8397	.1615	.1099	1.000	12.6
H33A	.5694	.0409	.0873	1.000	8.6
H33B	.4686	.0440	.1033	1.000	8.6
H34A	.5101	.1294	.0126	1.000	16.0
H34B	.5929	.1627	.0974	1.000	16.0
H34C	.4923	.1661	.1141	1.000	16.0
H35A	.3850	.0645	.3325	1.000	6.6
H35B	.3825	.0830	.2259	1.000	6.6
H36A	.3243	.1727	.3213	1.000	8.8
H36B	.4138	.2068	.2903	1.000	8.8
H36C	.4169	.1884	.3971	1.000	8.8
H37	.8005	.2213	.5679	1.000	3.8
H38	.6201	.2492	.5424	1.000	3.5
H40	.7105	.4035	.3215	1.000	5.0
H41	.8691	.3945	.3997	1.000	4.9
H45	1.0255	.3257	.7439	1.000	4.5
H46	.9820	.3480	.9088	1.000	4.7
H50	.6817	.4153	1.0460	1.000	5.6
H51	.5210	.4161	.9658	1.000	5.7
H55	.3360	.3513	.5920	1.000	5.0
H56	.3789	.3386	.4263	1.000	4.7
H60	.9374	.2511	.4450	1.000	5.2
H61	1.0684	.2558	.3720	1.000	6.5
H62	1.1874	.3527	.4254	1.000	6.7
H63	1.1772	.4416	.5536	1.000	7.8
H64	1.0473	.4369	.6294	1.000	6.4
H66	.7964	.2970	1.0486	1.000	10.8
H67	.8836	.3084	1.2092	1.000	11.8
H68	.9887	.4116	1.2742	1.000	7.4
H69	1.0068	.5020	1.1788	1.000	7.4
H70	.9226	.4896	1.0202	1.000	6.2
H72	.3909	.3014	.8557	1.000	5.9

Table II. Continued.

atom	x	y	z	occupancy	B(eq)
H73	.2513	.3141	.9112	1.000	7.3
H74	.1717	.4100	.8723	1.000	7.6
H75	.2322	.4940	.7837	1.000	7.4
H76	.3712	.4826	.7309	1.000	6.4
H78	.5780	.2886	.2455	1.000	5.4
H79	.5053	.3048	.0889	1.000	6.3
H80	.4087	.3930	.0715	1.000	6.2
H81	.3803	.4633	.2129	1.000	5.4
H82	.4551	.4497	.3695	1.000	4.5
CL3	1.2215(8)	.2760(7)	1.2035(9)	.400	22.2(4)
CL4	1.1253(9)	.3214(8)	1.075(1)	.400	25.7(5)
CL3'	1.1736(6)	.4040(5)	1.0871(7)	.300	11.9(2)
CL4'	1.208(1)	.2678(9)	1.109(2)	.300	21.3(6)
C83	1.171(1)	.345(1)	1.161(2)	.700	19.6(7)
H83A	1.2176	.3820	1.1547	.400	22.1
H83B	1.1321	.3607	1.2019	.400	22.1
H83C	1.2101	.3626	1.2208	.300	22.1
H83D	1.1095	.3314	1.1684	.300	22.1
CL5	1.246(1)	.2283(8)	1.051(1)	.300	18.9(5)
CL6	1.310(1)	.1474(9)	.967(1)	.300	27.9(7)
C84	1.287(1)	.174(1)	1.060(2)	.300	5.5(5)
H84A	1.2482	.1372	1.0793	.300	6.4
H84B	1.3422	.1881	1.1083	.300	6.4

Table III. Anisotropic thermal parameters for (**15b**)·CH_2Cl_2. 1/3

atom	U11	U22	U33	U12	U13	U23
Zn	.0458(4)	.0461(4)	.0495(5)	.0071(3)	.0202(4)	.0123(4)
Co	.0402(5)	.0441(5)	.0436(5)	.0053(4)	.0119(4)	.0090(4)
CL1	.059(1)	.048(1)	.079(1)	.0016(8)	.0202(9)	.0181(9)
CL2	.097(1)	.047(1)	.108(2)	.0074(9)	.056(1)	.025(1)
N1	.033(3)	.038(3)	.042(3)	.006(2)	.009(2)	.016(2)
N2	.039(3)	.040(3)	.041(3)	.012(2)	.013(2)	.005(2)
N3	.040(3)	.060(3)	.044(3)	.012(2)	.011(2)	.005(3)
N4	.046(3)	.055(3)	.034(3)	.001(2)	.012(2)	.009(2)
N5	.039(3)	.039(3)	.043(3)	.009(2)	.019(2)	.015(2)
N6	.037(3)	.042(3)	.042(3)	.004(2)	.011(2)	.013(2)
N7	.044(3)	.048(3)	.041(3)	.002(2)	.020(2)	.007(2)
N8	.039(3)	.041(3)	.037(3)	.011(2)	.012(2)	.006(2)
C1	.034(3)	.029(3)	.050(4)	.006(3)	.012(3)	.008(3)
C2	.039(3)	.038(3)	.051(4)	.006(3)	.017(3)	.008(3)
C3	.053(4)	.055(4)	.043(4)	.015(3)	.017(3)	.010(3)
C4	.047(4)	.040(3)	.035(3)	.009(3)	.008(3)	.004(3)
C5	.049(4)	.056(4)	.038(4)	.012(3)	.004(3)	.004(3)
C6	.038(3)	.040(3)	.052(4)	.008(3)	.009(3)	.011(3)
C7	.045(4)	.053(4)	.046(4)	.011(3)	.004(3)	.011(3)
C8	.038(4)	.048(4)	.063(4)	.010(3)	.010(3)	.019(3)
C9	.040(4)	.038(3)	.054(4)	.010(3)	.010(3)	.010(3)
C10	.041(4)	.055(4)	.067(5)	.019(3)	.020(3)	.018(4)
C11	.047(4)	.067(4)	.052(4)	.019(3)	.020(3)	.017(3)
C12	.053(4)	.125(6)	.059(5)	.040(4)	.024(4)	.022(4)
C13	.079(5)	.104(6)	.049(5)	.035(4)	.033(4)	.027(4)
C14	.052(4)	.067(4)	.053(4)	.013(3)	.019(4)	.009(4)
C15	.062(4)	.095(5)	.044(4)	.026(4)	.015(4)	.017(4)
C16	.046(4)	.072(5)	.049(4)	.011(3)	.009(3)	.014(4)
C17	.051(4)	.100(5)	.044(4)	.011(4)	.003(3)	.019(4)
C18	.041(4)	.066(4)	.055(4)	.008(3)	.006(3)	.014(3)
C19	.039(3)	.044(4)	.048(4)	.004(3)	.006(3)	.012(3)
C20	.028(3)	.042(3)	.052(4)	.003(3)	.010(3)	.009(3)
C21	.052(4)	.065(4)	.058(4)	.004(3)	.022(3)	.013(3)
C22	.063(5)	.119(7)	.184(9)	.022(5)	.051(5)	-.011(6)
C23	.057(4)	.125(7)	.052(5)	.006(5)	.018(4)	.017(5)
C24	.16(1)	.12(1)	.047(7)	-.029(8)	.030(7)	-.012(7)
C24'	.18(3)	.14(3)	.06(2)	-.03(2)	-.00(2)	.06(2)
C25	.052(4)	.090(5)	.071(5)	.020(4)	.004(4)	.019(4)
C26	.176(9)	.117(7)	.070(6)	.039(6)	.009(5)	.017(5)
C27	.044(4)	.088(5)	.070(5)	.022(4)	.009(3)	.016(4)
C28	.049(4)	.105(6)	.121(7)	-.002(4)	.015(4)	.023(5)
C29	.08(1)	.073(9)	.077(9)	-.000(9)	.027(7)	.019(9)

Table III. Continued.

atom	U11	U22	U33	U12	U13	U23
C29'	.03(2)	.09(3)	.06(2)	.02(2)	.04(1)	.03(2)
C30	.07(1)	.15(2)	.22(2)	.02(1)	.06(1)	.09(1)
C30'	.08(2)	.07(2)	.20(3)	.02(2)	.07(2)	-.07(2)
C31	.111(6)	.128(7)	.106(7)	.061(5)	.058(5)	.064(6)
C32	.126(7)	.20(1)	.099(7)	.056(7)	.053(6)	.058(7)
C33	.065(5)	.122(7)	.093(6)	.024(5)	.007(4)	.036(5)
C34	.26(1)	.16(1)	.101(8)	.057(9)	.043(8)	.038(7)
C35	.048(4)	.100(6)	.061(5)	.011(4)	.004(3)	.013(4)
C36	.067(5)	.103(6)	.120(7)	.024(4)	.020(5)	.038(5)
C37	.030(3)	.034(3)	.059(4)	.004(3)	.015(3)	.011(3)
C38	.035(3)	.037(3)	.042(3)	-.000(3)	.017(3)	.009(3)
C39	.049(4)	.046(4)	.037(4)	.013(3)	.015(3)	.017(3)
C40	.056(4)	.065(4)	.052(4)	.022(3)	.026(3)	.033(3)
C41	.046(4)	.062(4)	.057(4)	.012(3)	.027(3)	.022(3)
C42	.036(3)	.038(3)	.047(4)	.007(3)	.020(3)	.012(3)
C43	.035(3)	.035(3)	.052(4)	.001(3)	.013(3)	.007(3)
C44	.034(3)	.029(3)	.050(4)	-.001(2)	.011(3)	.002(3)
C45	.037(3)	.045(4)	.060(4)	.004(3)	.010(3)	.007(3)
C46	.052(4)	.044(4)	.049(4)	.003(3)	.007(3)	.001(3)
C47	.039(3)	.037(3)	.047(4)	-.001(3)	.005(3)	.008(3)
C48	.047(4)	.038(3)	.045(4)	-.001(3)	.006(3)	.010(3)
C49	.052(4)	.048(4)	.042(4)	.002(3)	.015(3)	.010(3)
C50	.064(4)	.075(5)	.036(4)	-.004(4)	.012(3)	.006(3)
C51	.053(4)	.072(5)	.055(5)	.000(3)	.025(4)	.001(4)
C52	.051(4)	.043(4)	.045(4)	.005(3)	.024(3)	.008(3)
C53	.044(4)	.044(4)	.043(4)	.005(3)	.017(3)	.007(3)
C54	.041(3)	.042(3)	.045(4)	.009(3)	.019(3)	.012(3)
C55	.039(4)	.069(4)	.055(4)	.010(3)	.023(3)	.011(3)
C56	.040(4)	.064(4)	.048(4)	.016(3)	.013(3)	.008(3)
C57	.038(3)	.045(3)	.043(4)	.012(3)	.012(3)	.013(3)
C58	.039(3)	.043(3)	.042(4)	.011(3)	.013(3)	.014(3)
C59	.036(3)	.049(4)	.052(4)	.003(3)	.016(3)	.010(3)
C60	.050(4)	.051(4)	.070(5)	.004(3)	.030(3)	.010(3)
C61	.072(5)	.071(5)	.073(5)	.022(4)	.037(4)	.009(4)
C62	.051(4)	.092(6)	.087(6)	.022(4)	.036(4)	.034(5)
C63	.053(4)	.081(6)	.114(7)	-.016(4)	.032(4)	.015(5)
C64	.054(4)	.062(4)	.082(5)	-.006(3)	.027(4)	-.007(4)
C65	.058(4)	.050(4)	.048(4)	.005(3)	.013(3)	.010(3)
C66	.165(8)	.085(6)	.061(5)	-.044(5)	-.034(5)	.024(5)
C67	.190(9)	.092(7)	.070(6)	-.023(6)	-.024(6)	.040(5)
C68	.091(6)	.087(6)	.047(5)	.015(5)	-.006(4)	-.006(4)
C69	.091(6)	.056(5)	.077(6)	.001(4)	.001(5)	.001(4)
C70	.074(5)	.060(5)	.059(5)	.006(4)	-.004(4)	.016(4)

atom	U11	U22	U33	U12	U13	U23
C71	.045(4)	.058(4)	.042(4)	.002(3)	.018(3)	.002(3)
C72	.054(4)	.080(5)	.052(4)	.002(4)	.021(3)	.005(4)
C73	.060(5)	.107(6)	.063(5)	-.013(4)	.035(4)	-.001(4)
C74	.045(4)	.115(7)	.077(6)	.004(4)	.029(4)	-.016(5)
C75	.063(5)	.087(6)	.092(6)	.025(4)	.030(4)	.000(4)
C76	.055(4)	.076(5)	.079(5)	.016(4)	.034(4)	.012(4)
C77	.041(3)	.048(4)	.043(4)	.011(3)	.014(3)	.013(3)
C78	.068(4)	.060(4)	.056(4)	.027(3)	.023(4)	.021(4)
C79	.093(5)	.075(5)	.035(4)	.020(4)	.016(4)	.008(4)
C80	.062(5)	.089(5)	.049(4)	.009(4)	.008(4)	.033(4)
C81	.055(4)	.068(5)	.058(5)	.019(3)	.013(4)	.030(4)
C82	.047(4)	.050(4)	.050(4)	.010(3)	.014(3)	.009(3)

Table IV. Bond distances for (15b)•CH_2Cl_2. 1/2

atom	atom	distance	atom	atom	distance	atom	atom	distance
Zn1	CL2	2.234(2)	C10	C11	1.387(7)	C52	C53	1.395(7)
Zn1	N5	2.559(4)	C11	C12	1.433(7)	C53	C54	1.381(6)
Zn1	N6	2.086(4)	C12	C13	1.357(7)	C53	C71	1.506(6)
Zn1	N7	2.016(4)	C12	C29	1.53(2)	C54	C55	1.446(7)
Zn1	N8	2.098(4)	C12	C29'	1.63(3)	C55	C56	1.339(6)
Co1	CL1	2.276(2)	C13	C14	1.460(7)	C56	C57	1.429(6)
Co1	N1	2.414(4)	C13	C31	1.526(8)	C57	C58	1.412(6)
Co1	N2	2.062(4)	C14	C15	1.382(7)	C58	C77	1.486(6)
Co1	N3	2.004(4)	C15	C16	1.403(7)	C59	C60	1.377(7)
Co1	N4	2.059(4)	C16	C17	1.451(7)	C59	C64	1.383(7)
N1	C1	1.419(5)	C17	C18	1.358(7)	C60	C61	1.387(7)
N1	C4	1.421(6)	C17	C33	1.555(8)	C61	C62	1.365(8)
N1	C37	1.460(5)	C18	C19	1.454(7)	C62	C63	1.352(8)
N2	C6	1.360(6)	C18	C35	1.499(7)	C63	C64	1.394(7)
N2	C9	1.386(6)	C19	C20	1.404(6)	C65	C66	1.358(8)
N3	C11	1.343(6)	C21	C22	1.505(8)	C65	C70	1.360(7)
N3	C14	1.376(6)	C23	C24	1.46(1)	C66	C67	1.402(9)
N4	C16	1.354(6)	C23	C24'	1.43(3)	C67	C68	1.350(8)
N4	C19	1.381(6)	C25	C26	1.484(8)	C68	C69	1.340(8)
N5	C38	1.451(5)	C27	C28	1.527(8)	C69	C70	1.373(8)
N5	C39	1.436(6)	C29	C30	1.38(2)	C71	C72	1.377(7)
N5	C42	1.412(5)	C29'	C30'	1.53(4)	C71	C76	1.377(7)
N6	C44	1.397(5)	C31	C32	1.47(1)	C72	C73	1.396(7)
N6	C47	1.373(6)	C33	C34	1.43(1)	C73	C74	1.382(8)
N7	C49	1.380(6)	C35	C36	1.525(8)	C74	C75	1.354(8)
N7	C52	1.369(6)	C37	C38	1.297(6)	C75	C76	1.380(7)
N8	C54	1.401(5)	C39	C40	1.407(6)	C77	C78	1.391(7)
N8	C57	1.366(6)	C39	C58	1.379(6)	C77	C82	1.391(6)
C1	C2	1.405(6)	C40	C41	1.358(7)	C78	C79	1.382(7)
C1	C20	1.375(6)	C41	C42	1.404(6)	C79	C80	1.369(7)
C2	C3	1.379(7)	C42	C43	1.394(6)	C80	C81	1.376(7)
C2	C21	1.497(6)	C43	C44	1.385(6)	C81	C82	1.380(7)
C3	C4	1.424(6)	C43	C59	1.490(6)			
C3	C23	1.505(7)	C44	C45	1.436(6)	CL3	C83	1.69(2)
C4	C5	1.372(6)	C45	C46	1.340(7)	CL4	C83	1.25(2)
C5	C6	1.412(6)	C46	C47	1.425(7)	CL3'	C83	1.60(2)
C6	C7	1.442(6)	C47	C48	1.416(7)	CL4'	C83	1.71(2)
C7	C8	1.357(7)	C48	C49	1.376(6)			
C7	C25	1.505(7)	C48	C65	1.494(7)	CL5	C84	1.25(2)
C8	C9	1.454(7)	C49	C50	1.448(7)	CL6	C84	1.42(2)
C8	C27	1.504(7)	C50	C51	1.339(7)			
C9	C10	1.395(7)	C51	C52	1.429(7)			

Table IV. Continued.

atom	atom	distance
C5	H5	0.952
C10	H10	0.949
C15	H15	0.952
C20	H20	0.950
C21	H21A	0.950
C21	H21B	0.952
C22	H22A	0.944
C22	H22B	0.954
C22	H22C	0.950
C23	H23A	0.955
C23	H23B	0.954
C23	H23C	0.949
C23	H23D	0.945
C24	H24A	0.931
C24	H24B	0.946
C24	H24C	0.944
C24'	H24D	0.959
C24'	H24E	0.950
C24'	H24F	0.897
C25	H25A	0.951
C25	H25B	0.951
C26	H26A	0.948
C26	H26B	0.948
C26	H26C	0.953
C27	H27A	0.951
C27	H27B	0.950
C28	H28A	0.949
C28	H28B	0.950
C28	H28C	0.947
C29	H29A	0.940
C29	H29B	0.953
C29'	H29C	1.257
C29'	H29D	1.029
C30	H30A	0.930
C30	H30B	1.024
C30	H30C	1.001
C30'	H30D	1.079
C30'	H30E	0.879
C30'	H30F	0.934
C31	H31A	0.952
C31	H31B	0.951
C32	H32A	0.951
C32	H32B	0.947
C32	H32C	0.953
C33	H33A	0.949
C33	H33B	0.949
C34	H34A	0.944
C34	H34B	0.957
C34	H34C	0.951
C35	H35A	0.951
C35	H35B	0.951
C36	H36A	0.952
C36	H36B	0.950
C36	H36C	0.951
C37	H37	0.951
C38	H38	0.950
C40	H40	0.948
C41	H41	0.951
C45	H45	0.951
C46	H46	0.950
C50	H50	0.952
C51	H51	0.949
C55	H55	0.948
C56	H56	0.951
C60	H60	0.949
C61	H61	0.950
C62	H62	0.950
C63	H63	0.951
C64	H64	0.951
C66	H66	0.949
C67	H67	0.952
C68	H68	0.950
C69	H69	0.948
C70	H70	0.948
C72	H72	0.950
C73	H73	0.948
C74	H74	0.950
C75	H75	0.953
C76	H76	0.950
C78	H78	0.951
C79	H79	0.950
C80	H80	0.949
C81	H81	0.950
C82	H82	0.950
C83	H83A	0.939
C83	H83B	0.921
C83	H83C	0.926
C83	H83D	0.944
C84	H84A	0.943
C84	H84B	0.948

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table V. Bond angles for (15b)•CH_2Cl_2. 1/3

atom	atom	atom	angle	atom	atom	atom	angle	atom	atom	atom	angle
CL2	Zn	N5	92.4(1)	Zn	N7	C49	123.6(3)	N3	C14	C15	124.5(5)
CL2	Zn	N6	103.1(1)	Zn	N7	C52	125.2(4)	C13	C14	C15	126.4(6)
CL2	Zn	N7	124.1(1)	C49	N7	C52	108.1(4)	C14	C15	C16	126.5(6)
CL2	Zn	N8	105.8(1)	Zn	N8	C54	121.3(3)	N4	C16	C15	125.8(5)
N5	Zn	N6	81.3(1)	Zn	N8	C57	131.9(3)	N4	C16	C17	111.0(5)
N5	Zn	N7	143.6(1)	C54	N8	C57	105.6(4)	C15	C16	C17	123.2(6)
N5	Zn	N8	79.1(1)	N1	C1	C2	108.7(5)	C16	C17	C18	107.3(5)
N6	Zn	N7	89.3(2)	N1	C1	C20	123.0(5)	C16	C17	C33	125.4(5)
N6	Zn	N8	145.5(2)	C2	C1	C20	128.3(5)	C18	C17	C33	127.1(6)
N7	Zn	N8	89.9(2)	C1	C2	C3	108.2(5)	C17	C18	C19	105.4(5)
CL1	Co	N1	93.8(1)	C1	C2	C21	124.6(5)	C17	C18	C35	129.5(6)
CL1	Co	N2	104.9(1)	C3	C2	C21	127.2(5)	C19	C18	C35	125.1(5)
CL1	Co	N3	118.7(1)	C2	C3	C4	108.9(5)	N4	C19	C18	111.1(5)
CL1	Co	N4	103.7(1)	C2	C3	C23	127.3(5)	N4	C19	C20	125.6(5)
N1	Co	N2	81.8(1)	C4	C3	C23	123.8(5)	C18	C19	C20	123.1(5)
N1	Co	N3	147.4(2)	N1	C4	C3	107.2(5)	C1	C20	C19	126.8(5)
N1	Co	N4	80.7(2)	N1	C4	C5	124.3(5)	C2	C21	C22	111.9(5)
N2	Co	N3	89.4(2)	C3	C4	C5	128.4(5)	C3	C23	C24	110.9(7)
N2	Co	N4	147.1(2)	C4	C5	C6	127.1(5)	C3	C23	C24'	118(1)
N3	Co	N4	90.6(2)	N2	C6	C5	124.5(5)	C7	C25	C26	113.6(6)
Co	N1	C1	114.7(3)	N2	C6	C7	112.4(5)	C8	C27	C28	112.3(5)
Co	N1	C4	114.6(3)	C5	C6	C7	123.0(5)	C12	C29	C30	107(2)
Co	N1	C37	91.9(3)	C6	C7	C8	106.1(5)	C12	C29'	C30'	111(3)
C1	N1	C4	106.7(4)	C6	C7	C25	126.9(5)	C13	C31	C32	108.3(7)
C1	N1	C37	117.8(4)	C8	C7	C25	127.0(5)	C17	C33	C34	108.5(7)
C4	N1	C37	110.9(4)	C7	C8	C9	106.5(5)	C18	C35	C36	112.9(5)
Co	N2	C6	132.0(3)	C7	C8	C27	128.5(6)	N1	C37	C38	124.7(4)
Co	N2	C9	122.4(4)	C9	C8	C27	124.8(5)	N5	C38	C37	123.9(4)
C6	N2	C9	104.3(4)	N2	C9	C8	110.7(5)	N5	C39	C40	105.4(4)
Co	N3	C11	127.4(4)	N2	C9	C10	125.5(5)	N5	C39	C58	125.6(4)
Co	N3	C14	126.1(4)	C8	C9	C10	123.8(5)	C40	C39	C58	128.7(5)
C11	N3	C14	106.3(5)	C9	C10	C11	126.5(5)	C39	C40	C41	109.9(5)
Co	N4	C16	123.4(4)	N3	C11	C10	123.4(5)	C40	C41	C42	109.7(5)
Co	N4	C19	129.0(4)	N3	C11	C12	111.5(5)	N5	C42	C41	106.3(4)
C16	N4	C19	105.3(4)	C10	C11	C12	124.8(6)	N5	C42	C43	126.5(5)
Zn	N5	C38	90.9(3)	C11	C12	C13	106.4(5)	C41	C42	C43	126.6(5)
Zn	N5	C39	107.3(3)	C11	C12	C29	126.4(8)	C42	C43	C44	126.0(5)
Zn	N5	C42	107.4(3)	C11	C12	C29'	122(1)	C42	C43	C59	112.6(5)
C38	N5	C39	117.9(4)	C13	C12	C29	125.8(8)	C44	C43	C59	121.1(5)
C38	N5	C42	121.8(4)	C13	C12	C29'	125(1)	N6	C44	C43	126.3(5)
C39	N5	C42	108.5(4)	C12	C13	C14	106.5(6)	N6	C44	C45	108.5(5)
Zn	N6	C44	129.6(3)	C12	C13	C31	130.7(6)	C43	C44	C45	125.0(5)
Zn	N6	C47	122.6(3)	C14	C13	C31	122.8(6)	C44	C45	C46	107.8(5)
C44	N6	C47	106.0(4)	N3	C14	C13	109.2(5)	C45	C46	C47	107.6(5)

Table V. Continued.

atom	atom	atom	angle	atom	atom	atom	angle	atom	atom	atom	angle
N6	C47	C46	109.9(5)	C53	C71	C72	120.5(5)	C24'	C23	H23C	107.83
N6	C47	C48	125.8(5)	C53	C71	C76	120.9(5)	C24'	C23	H23D	105.51
C46	C47	C48	124.3(5)	C72	C71	C76	118.6(5)	H23A	C23	H23B	108.70
C47	C48	C49	125.3(5)	C71	C72	C73	120.4(6)	H23C	C23	H23D	109.99
C47	C48	C65	117.0(5)	C72	C73	C74	119.5(6)	C23	C24	H24A	108.50
C49	C48	C65	117.7(5)	C73	C74	C75	120.1(6)	C23	C24	H24B	107.28
N7	C49	C48	25.5(5)	C74	C75	C76	120.3(6)	C23	C24	H24C	107.41
N7	C49	C50	107.8(5)	C71	C76	C75	121.1(6)	H24A	C24	H24B	111.48
C48	C49	C50	126.6(6)	C58	C77	C78	120.9(5)	H24A	C24	H24C	111.65
C49	C50	C51	107.2(5)	C58	C77	C82	121.7(5)	H24B	C24	H24C	110.31
C50	C51	C52	108.7(5)	C78	C77	C82	117.4(5)	C23	C24'	H24D	105.27
N7	C52	C51	108.1(5)	C77	C78	C79	120.7(5)	C23	C24'	H24E	105.79
N7	C52	C53	124.1(5)	C78	C79	C80	120.9(6)	C23	C24'	H24F	108.89
C51	C52	C53	127.7(5)	C79	C80	C81	119.3(6)	H24D	C24'	H24E	108.70
C52	C53	C54	126.3(5)	C80	C81	C82	120.1(5)	H24D	C24'	H24F	113.36
C52	C53	C71	116.7(5)	C77	C82	C81	121.5(5)	H24E	C24'	H24F	114.19
C54	C53	C71	117.0(5)	CL3	C83	CL4	108(2)	C7	C25	H25A	108.15
N8	C54	C53	127.1(5)	CL3'	C83	CL4'	110(2)	C7	C25	H25B	108.21
N8	C54	C55	108.7(5)	CL5	C84	CL6	109(2)	C26	C25	H25A	108.76
C53	C54	C55	124.2(5)	C4	C5	H5	116.52	C26	C25	H25B	108.72
C54	C55	C56	107.5(5)	C6	C5	H5	116.36	H25A	C25	H25B	109.31
C55	C56	C57	107.5(5)	C9	C10	H10	116.76	C25	C26	H26A	109.47
N8	C57	C56	110.6(4)	C11	C10	H10	116.74	C25	C26	H26B	109.50
N8	C57	C58	125.1(5)	C14	C15	H15	116.79	C25	C26	H26C	109.13
C56	C57	C58	124.3(5)	C16	C15	H15	116.67	H26A	C26	H26B	109.85
C39	C58	C57	125.1(5)	C1	C20	H20	116.74	H26A	C26	H26C	109.43
C39	C58	C77	115.8(4)	C19	C20	H20	116.50	H26B	C26	H26C	109.44
C57	C58	C77	118.8(5)	C2	C21	H21A	109.02	C8	C27	H27A	108.71
C43	C59	C60	120.4(5)	C2	C21	H21B	108.63	C8	C27	H27B	108.73
C43	C59	C64	121.9(5)	C22	C21	H21A	108.89	C28	C27	H27A	108.77
C60	C59	C64	117.5(5)	C22	C21	H21B	109.00	C28	C27	H27B	108.96
C59	C60	C61	121.7(5)	H21A	C21	H21B	109.33	H27A	C27	H27B	109.34
C60	C61	C62	119.9(6)	C21	C22	H22A	109.62	C27	C28	H28A	109.14
C61	C62	C63	119.6(6)	C21	C22	H22B	109.10	C27	C28	H28B	109.14
C62	C63	C64	121.1(6)	C21	C22	H22C	109.32	C27	C28	H28C	109.35
C59	C64	C63	120.3(6)	H22A	C22	H22B	109.67	H28A	C28	H28B	109.56
C48	C65	C66	122.1(6)	H22A	C22	H22C	109.99	H28A	C28	H28C	109.85
C48	C65	C70	121.9(5)	H22B	C22	H22C	109.12	H28B	C28	H28C	109.78
C66	C65	C70	115.9(6)	C3	C23	H23A	109.06	C12	C29	H29A	109.71
C65	C66	C67	121.6(7)	C3	C23	H23B	109.39	C12	C29	H29B	109.21
C66	C67	C68	120.2(7)	C3	C23	H23C	107.82	C30	C29	H29A	111.71
C67	C68	C69	118.7(7)	C3	C23	H23D	107.77	C30	C29	H29B	108.85
C68	C69	C70	120.6(6)	C24	C23	H23A	109.29	H29A	C29	H29B	110.10
C65	C70	C69	122.8(6)	C24	C23	H23B	109.49	C29	C30	H30A	118.16

atom	atom	atom	angle	atom	atom	atom	angle	atom	atom	atom	angle
C29	C30	H30B	111.67	C35	C36	H36B	109.60	C69	C70	H70	118.72
C29	C30	H30C	113.99	C35	C36	H36C	109.58	C71	C72	H72	120.01
H30A	C30	H30B	105.07	H36A	C36	H36B	109.34	C73	C72	H72	119.60
H30A	C30	H30C	103.69	H36A	C36	H36C	109.29	C72	C73	H73	120.54
H30B	C30	H30C	102.72	H36B	C36	H36C	109.43	C74	C73	H73	119.92
C12	C29'	H29C	114.72	N1	C37	H37	117.66	C73	C74	H74	120.21
C12	C29'	H29D	120.13	C38	C37	H37	117.61	C75	C74	H74	119.69
C30'	C29'	H29C	103.62	N5	C38	H38	118.12	C74	C75	H75	120.19
C30'	C29'	H29D	103.95	C37	C38	H38	117.99	C76	C75	H75	119.56
H29C	C29'	H29D	101.52	C39	C40	H40	124.93	C71	C76	H76	119.35
C29'	C30'	H30D	82.53	C41	C40	H40	125.14	C75	C76	H76	119.51
C29'	C30'	H30E	94.19	C40	C41	H41	125.13	C77	C78	H78	119.47
C29'	C30'	H30F	145.53	C42	C41	H41	125.15	C79	C78	H78	119.80
H30D	C30'	H30E	104.34	C44	C45	H45	126.02	C78	C79	H79	119.55
H30D	C30'	H30F	100.58	C46	C45	H45	126.14	C80	C79	H79	119.54
H30E	C30'	H30F	117.64	C45	C46	H46	126.18	C79	C80	H80	120.35
C13	C31	H31A	109.70	C47	C46	H46	126.17	C81	C80	H80	120.33
C13	C31	H31B	109.83	C49	C50	H50	126.25	C80	C81	H81	120.02
C32	C31	H31A	109.72	C51	C50	H50	126.58	C82	C81	H81	119.89
C32	C31	H31B	110.00	C50	C51	H51	125.42	C77	C82	H82	119.19
H31A	C31	H31B	109.26	C52	C51	H51	125.84	C81	C82	H82	119.32
C31	C32	H32A	109.52	C54	C55	H55	126.29				
C31	C32	H32B	109.73	C56	C55	H55	126.18	CL3	C83	H83A	108.73
C31	C32	H32C	109.35	C55	C56	H56	126.25	CL3	C83	H83B	109.70
H32A	C32	H32B	109.60	C57	C56	H56	126.30	CL4	C83	H83A	107.70
H32A	C32	H32C	109.13	C59	C60	H60	119.08	CL4	C83	H83B	109.54
H32B	C32	H32C	109.50	C61	C60	H60	119.26	H83A	C83	H83B	113.04
C17	C33	H33A	109.90	C60	C61	H61	120.09	CL3'	C83	H83C	110.58
C17	C33	H33B	109.91	C62	C61	H61	120.05	CL3'	C83	H83D	109.79
C34	C33	H33A	109.57	C61	C62	H62	120.47	CL4'	C83	H83C	107.96
C34	C33	H33B	109.37	C63	C62	H62	119.96	CL4'	C83	H83D	106.63
H33A	C33	H33B	109.61	C62	C63	H63	119.67	H83C	C83	H83D	112.12
C33	C34	H34A	110.03	C64	C63	H63	119.28				
C33	C34	H34B	109.21	C59	C64	H64	119.69	CL5	C84	H84A	109.48
C33	C34	H34C	109.55	C63	C64	H64	120.00	CL5	C84	H84B	109.31
H34A	C34	H34B	109.37	C65	C66	H66	119.15	CL6	C84	H84A	109.24
H34A	C34	H34C	109.87	C67	C66	H66	119.28	CL6	C84	H84B	109.51
H34B	C34	H34C	108.79	C66	C67	H67	119.89	H84A	C84	H84B	110.23
C18	C35	H35A	108.62	C68	C67	H67	119.87				
C18	C35	H35B	108.71	C67	C68	H68	120.58				
C36	C35	H35A	108.65	C69	C68	H68	120.75				
C36	C35	H35B	108.64	C68	C69	H69	119.65				
H35A	C35	H35B	109.31	C70	C69	H69	119.71				
C35	C36	H36A	109.58	C65	C70	H70	118.50				

Angles are in degrees.
Estimated standard deviations in the least significant figure are given in parentheses.

Table VI. Torsion angles for (15b)•CH_2Cl_2.

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
Zn	N5	C38	C37	-108.3(5)	CL2	Zn	N5	C38	-178.0(3)
Zn	N5	C39	C40	119.8(4)	CL2	Zn	N5	C39	-58.4(3)
Zn	N5	C39	C58	-54.2(6)	CL2	Zn	N5	C42	58.1(3)
Zn	N5	C42	C41	-119.8(4)	CL2	Zn	N6	C44	-61.0(4)
Zn	N5	C42	C43	51.5(6)	CL2	Zn	N6	C47	101.4(4)
Zn	N6	C44	C43	-9.1(7)	CL2	Zn	N7	C49	-75.7(4)
Zn	N6	C44	C45	167.0(3)	CL2	Zn	N7	C52	81.9(4)
Zn	N6	C47	C46	-168.2(3)	CL2	Zn	N8	C54	-107.5(3)
Zn	N6	C47	C48	11.4(7)	CL2	Zn	N8	C57	58.0(4)
Zn	N7	C49	C48	-24.3(7)	N1	Co	N2	C6	25.7(4)
Zn	N7	C49	C50	158.8(3)	N1	Co	N2	C9	-169.9(4)
Zn	N7	C52	C51	-158.3(4)	N1	Co	N3	C11	96.5(5)
Zn	N7	C52	C53	24.3(7)	N1	Co	N3	C14	-88.7(5)
Zn	N8	C54	C53	-6.0(7)	N1	Co	N4	C16	166.9(4)
Zn	N8	C54	C55	172.7(3)	N1	Co	N4	C19	-33.1(4)
Zn	N8	C57	C56	-171.0(3)	N2	Co	N1	C1	-162.7(3)
Zn	N8	C57	C58	8.5(8)	N2	Co	N1	C4	-38.8(3)
Co	N1	C1	C2	134.0(3)	N2	Co	N1	C37	75.3(3)
Co	N1	C1	C20	-42.9(6)	N2	Co	N3	C11	22.8(5)
Co	N1	C4	C3	-134.4(3)	N2	Co	N3	C14	-162.4(5)
Co	N1	C4	C5	42.9(6)	N2	Co	N4	C16	108.4(5)
Co	N1	C37	C38	128.6(5)	N2	Co	N4	C19	-91.6(5)
Co	N2	C6	C5	-9.0(8)	N3	Co	N1	C1	121.4(4)
Co	N2	C6	C7	167.8(3)	N3	Co	N1	C4	-114.6(4)
Co	N2	C9	C8	-168.9(3)	N3	Co	N1	C37	-0.5(4)
Co	N2	C9	C10	11.8(7)	N3	Co	N2	C6	174.2(5)
Co	N3	C11	C10	-12.9(8)	N3	Co	N2	C9	-21.4(4)
Co	N3	C11	C12	172.4(4)	N3	Co	N4	C16	18.4(4)
Co	N3	C14	C13	-173.7(4)	N3	Co	N4	C19	178.4(4)
Co	N3	C14	C15	6.7(9)	N4	Co	N1	C1	45.1(3)
Co	N4	C16	C15	-14.0(8)	N4	Co	N1	C4	169.1(3)
Co	N4	C16	C17	164.0(4)	N4	Co	N1	C37	-76.8(3)
Co	N4	C19	C18	-162.5(4)	N4	Co	N2	C6	83.9(5)
Co	N4	C19	C20	13.5(8)	N4	Co	N2	C9	-111.6(4)
CL1	Co	N1	C1	-58.2(3)	N4	Co	N3	C11	170.0(5)
CL1	Co	N1	C4	65.8(3)	N4	Co	N3	C14	-15.2(5)
CL1	Co	N1	C37	179.9(3)	N5	Zn	N6	C44	29.4(4)
CL1	Co	N2	C6	-66.1(4)	N5	Zn	N6	C47	-168.2(4)
CL1	Co	N2	C9	98.3(4)	N5	Zn	N7	C49	103.9(4)
CL1	Co	N3	C11	-84.0(5)	N5	Zn	N7	C52	-98.5(4)
CL1	Co	N3	C14	90.9(5)	N5	Zn	N8	C54	163.1(4)
CL1	Co	N4	C16	-101.4(4)	N5	Zn	N8	C57	-31.4(4)
CL1	Co	N4	C19	58.6(4)	N6	Zn	N5	C38	79.2(3)

Table VI. Continued.

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
N6	Zn	N5	C39	-161.2(3)	N4	C19	C18	C17	-0.6(7)
N6	Zn	N5	C42	-44.7(3)	N4	C19	C18	C35	-179.9(5)
N6	Zn	N7	C49	29.7(4)	N4	C19	C20	C1	11.0(9)
N6	Zn	N7	C52	-172.7(4)	N5	C39	C40	C41	-2.4(6)
N6	Zn	N8	C54	106.8(4)	N5	C39	C58	C57	22.4(9)
N6	Zn	N8	C57	-87.7(5)	N5	C39	C58	C77	-163.8(5)
N7	Zn	N5	C38	2.3(4)	N5	C42	C41	C40	2.7(6)
N7	Zn	N5	C39	122.0(3)	N5	C42	C43	C44	-23.3(8)
N7	Zn	N5	C42	-121.6(3)	N5	C42	C43	C59	162.7(5)
N7	Zn	N6	C44	174.1(4)	N6	C44	C43	C42	-8.4(8)
N7	Zn	N6	C47	-23.6(4)	N6	C44	C43	C59	165.3(5)
N7	Zn	N8	C54	18.1(4)	N6	C44	C45	C46	-1.5(6)
N7	Zn	N8	C57	-176.4(4)	N6	C47	C46	C45	1.4(6)
N8	Zn	N5	C38	-72.4(3)	N6	C47	C48	C49	5.4(9)
N8	Zn	N5	C39	47.3(3)	N6	C47	C48	C65	-174.9(5)
N8	Zn	N5	C42	163.7(3)	N7	C49	C48	C47	1.2(9)
N8	Zn	N6	C44	85.1(5)	N7	C49	C48	C65	-178.4(5)
N8	Zn	N6	C47	-112.5(4)	N7	C49	C50	C51	1.3(7)
N8	Zn	N7	C49	175.2(4)	N7	C52	C51	C50	-1.4(7)
N8	Zn	N7	C52	-27.2(4)	N7	C52	C53	C54	-2.8(9)
N1	C1	C2	C3	-3.2(6)	N7	C52	C53	C71	177.3(5)
N1	C1	C2	C21	176.7(4)	N8	C54	C53	C52	-6.5(9)
N1	C1	C20	C19	10.2(8)	N8	C54	C53	C71	173.4(5)
N1	C4	C3	C2	4.4(6)	N8	C54	C55	C56	-2.6(6)
N1	C4	C3	C23	-178.8(6)	N8	C57	C56	C55	2.3(6)
N1	C4	C5	C6	-17.3(9)	N8	C57	C58	C39	11.1(9)
N1	C37	C38	N5	179.3(4)	N8	C57	C58	C77	-162.5(5)
N2	C6	C5	C4	-5.9(9)	C1	N1	C4	C3	-6.2(5)
N2	C6	C7	C8	-1.5(6)	C1	N1	C4	C5	171.1(5)
N2	C6	C7	C25	177.1(5)	C1	N1	C37	C38	9.2(8)
N2	C9	C8	C7	-0.1(6)	C1	C2	C3	C4	-0.7(6)
N2	C9	C8	C27	-174.5(5)	C1	C2	C3	C23	-177.4(6)
N2	C9	C10	C11	7.3(9)	C1	C2	C21	C22	-88.1(7)
N3	C11	C10	C9	-7(1)	C1	C20	C19	C18	-173.5(5)
N3	C11	C12	C13	3.2(8)	C2	C1	N1	C4	5.9(5)
N3	C11	C12	C29	-163.9(8)	C2	C1	N1	C37	-119.6(5)
N3	C11	C12	C29'	157(2)	C2	C1'	C20	C19	-166.1(5)
N3	C14	C13	C12	-0.1(8)	C2	C3	C4	C5	-172.8(5)
N3	C14	C13	C31	-178.2(6)	C2	C3	C23	C24	-97.0(8)
N3	C14	C15	C16	6(1)	C2	C3	C23	C24'	103(1)
N4	C16	C15	C14	-1(1)	C3	C2	C1	C20	173.5(5)
N4	C16	C17	C18	-0.4(7)	C3	C2	C21	C22	91.8(7)
N4	C16	C17	C33	-175.7(6)	C3	C4	N1	C37	123.3(4)

Table VI. Continued.

(1)	(2)	(3)	(4)	angle
C3	C4	C5	C6	159.4(5)
C4	N1	C1	C20	-171.0(5)
C4	N1	C37	C38	-114.1(6)
C4	C3	C2	C21	179.3(5)
C4	C3	C23	C24	86.8(8)
C4	C3	C23	C24'	-73(1)
C4	C5	C6	C7	177.5(5)
C5	C4	N1	C37	-59.4(6)
C5	C4	C3	C23	4.0(9)
C5	C6	N2	C9	-175.5(5)
C5	C6	C7	C8	175.4(5)
C5	C6	C7	C25	-5.9(9)
C6	N2	C9	C8	-0.8(6)
C6	N2	C9	C10	179.9(5)
C6	C7	C8	C9	0.9(6)
C6	C7	C8	C27	175.1(5)
C6	C7	C25	C26	96.2(7)
C7	C6	N2	C9	1.4(6)
C7	C8	C9	C10	179.2(5)
C7	C8	C27	C28	-98.1(7)
C8	C7	C25	C26	-85.5(8)
C8	C9	C10	C11	-172.0(5)
C9	C8	C7	C25	-177.7(5)
C9	C8	C27	C28	75.0(7)
C9	C10	C11	C12	166.6(6)
C10	C9	C8	C27	4.8(9)
C10	C11	N3	C14	171.4(5)
C10	C11	C12	C13	-171.4(6)
C10	C11	C12	C29	21(1)
C10	C11	C12	C29'	-18(2)
C11	N3	C14	C13	2.1(7)
C11	N3	C14	C15	-177.6(6)
C11	C12	C13	C14	-1.8(8)
C11	C12	C13	C31	176.1(7)
C11	C12	C29	C30	-101(1)
C11	C12	C29'	C30'	126(2)
C12	C11	N3	C14	-3.3(7)
C12	C13	C14	C15	179.5(6)
C12	C13	C31	C32	-96.2(9)
C13	C12	C29	C30	94(2)
C13	C12	C29'	C30'	-86(3)
C13	C14	C15	C16	-174.1(6)
C14	C13	C12	C29	165.5(8)
C14	C13	C12	C29'	-154(2)
C14	C13	C31	C32	81.3(9)
C14	C15	C16	C17	-179.0(6)
C15	C14	C13	C31	2(1)
C15	C16	N4	C19	-178.0(6)
C15	C16	C17	C18	177.7(6)
C15	C16	C17	C33	2(1)
C16	N4	C19	C18	0.3(6)
C16	N4	C19	C20	176.3(5)
C16	C17	C18	C19	0.5(7)
C16	C17	C18	C35	179.8(6)
C16	C17	C33	C34	-94.8(9)
C17	C16	N4	C19	0.0(6)
C17	C18	C19	C20	-176.7(5)
C17	C18	C35	C36	-109.9(8)
C18	C17	C33	C34	90.8(9)
C19	C18	C17	C33	175.7(6)
C19	C18	C35	C36	69.2(8)
C20	C1	N1	C37	63.6(6)
C20	C1	C2	C21	-6.6(9)
C20	C19	C18	C35	4.0(9)
C21	C2	C3	C23	3(1)
C25	C7	C8	C27	-4(1)
C29	C12	C13	C31	-17(1)
C31	C13	C12	C29'	24(2)
C33	C17	C18	C35	-5(1)
C37	C38	N5	C39	141.6(5)
C37	C38	N5	C42	3.0(8)
C38	N5	C39	C40	-139.6(4)
C38	N5	C39	C58	46.4(7)
C38	N5	C42	C41	137.8(5)
C38	N5	C42	C43	-50.9(7)
C39	N5	C42	C41	-4.1(6)
C39	N5	C42	C43	167.2(5)
C39	C40	C41	C42	-0.1(7)
C39	C58	C57	C56	-169.5(5)
C39	C58	C77	C78	47.7(7)
C39	C58	C77	C82	-130.3(5)
C40	C39	N5	C42	4.1(6)
C40	C39	C58	C57	-150.2(6)
C40	C39	C58	C77	23.7(8)
C40	C41	C42	C43	-168.7(5)
C41	C40	C39	C58	171.3(6)

Table VI. Continued.

(1)	(2)	(3)	(4)	angle
C41	C42	C43	C44	146.4(6)
C41	C42	C43	C59	-27.7(8)
C42	N5	C39	C58	-169.9(5)
C42	C43	C44	C45	176.2(5)
C42	C43	C59	C60	-58.7(7)
C42	C43	C59	C64	116.5(6)
C43	C44	N6	C47	-173.7(5)
C43	C44	C45	C46	174.6(5)
C43	C59	C60	C61	174.6(5)
C43	C59	C64	C63	-173.9(6)
C44	N6	C47	C46	-2.3(6)
C44	N6	C47	C48	177.3(5)
C44	C43	C59	C60	126.9(6)
C44	C43	C59	C64	-57.9(8)
C44	C45	C46	C47	0.1(6)
C45	C44	N6	C47	2.3(5)
C45	C44	C43	C59	-10.2(8)
C45	C46	C47	C48	-178.2(5)
C46	C47	C48	C49	-175.1(5)
C46	C47	C48	C65	4.6(8)
C47	C48	C49	C50	177.5(5)
C47	C48	C65	C66	-106.3(7)
C47	C48	C65	C70	78.0(7)
C48	C49	N7	C52	174.7(5)
C48	C49	C50	C51	-175.6(5)
C48	C65	C66	C67	179.1(7)
C48	C65	C70	C69	-179.5(6)
C49	N7	C52	C51	2.2(6)
C49	N7	C52	C53	-175.2(5)
C49	C48	C65	C66	73.4(8)
C49	C48	C65	C70	-102.3(7)
C49	C50	C51	C52	0.1(7)
C50	C49	N7	C52	-2.1(6)
C50	C49	C48	C65	-2.1(8)
C50	C51	C52	C53	175.9(5)
C51	C52	C53	C54	-179.6(5)
C51	C52	C53	C71	0.5(9)
C52	C53	C54	C55	174.9(5)
C52	C53	C71	C72	-65.9(7)
C52	C53	C71	C76	114.1(6)
C53	C54	N8	C57	-174.9(5)
C53	C54	C55	C56	176.2(5)
C53	C71	C72	C73	179.9(5)
C53	C71	C76	C75	179.9(6)
C54	N8	C57	C56	-3.8(6)
C54	N8	C57	C58	175.6(5)
C54	C53	C71	C72	114.1(6)
C54	C53	C71	C76	-65.8(7)
C54	C55	C56	C57	0.2(6)
C55	C54	N8	C57	3.9(6)
C55	C54	C53	C71	-5.2(8)
C55	C56	C57	C58	-177.2(5)
C56	C57	C58	C77	16.8(8)
C57	C58	C77	C78	-138.0(5)
C57	C58	C77	C82	43.9(7)
C58	C77	C78	C79	-179.3(5)
C58	C77	C82	C81	-179.9(5)
C59	C60	C61	C62	0(1)
C59	C64	C63	C62	-1(1)
C60	C59	C64	C63	1.5(9)
C60	C61	C62	C63	1(1)
C61	C60	C59	C64	-0.9(9)
C61	C62	C63	C64	0(1)
C65	C66	C67	C68	3(1)
C65	C70	C69	C68	-2(1)
C66	C65	C70	C69	5(1)
C66	C67	C68	C69	1(1)
C67	C66	C65	C70	-5(1)
C67	C68	C69	C70	-1(1)
C71	C72	C73	C74	0(1)
C71	C76	C75	C74	0(1)
C72	C71	C76	C75	-0.1(9)
C72	C73	C74	C75	0(1)
C73	C72	C71	C76	-0.1(9)
C73	C74	C75	C76	0(1)
C77	C78	C79	C80	1(1)
C77	C82	C81	C80	-2.3(9)
C78	C77	C82	C81	2.0(8)
C78	C79	C80	C81	-1(1)
C79	C78	C77	C82	-1.2(8)
C79	C80	C81	C82	1.8(9)

The sign is positive if when looking from atom 2 to atom 3 a clock-wise motion of atom 1 would superimpose it on atom 4.

Table VII. Least-squares planes for (15b)•CH_2Cl_2.

---------- Plane number 1 ----------

Atoms Defining Plane	Distance	esd
N(2) (1)	.0000	
N(3) (1)	.0000	
N(4) (1)	.0000	

Additional Atoms	Distance
Co(1) (1)	.5593

Mean deviation from plane is .0000 angstroms
Chi-squared: .0

---------- Plane number 2 ----------

Atoms Defining Plane	Distance	esd
N(6) (1)	.0000	
N(7) (1)	.0000	
N(8) (1)	.0000	

Additional Atoms	Distance
Zn(1) (1)	.5962

Mean deviation from plane is .0000 angstroms
Chi-squared: .0

Dihedral angles between least-squares planes

plane	plane	angle
2	1	174.21

---------- Plane number 3 ----------

Atoms Defining Plane	Distance	esd
N(1) (1)	-.0267	.0037
C(1) (1)	.0303	.0046
C(2) (1)	-.0103	.0048
C(3) (1)	-.0177	.0052
C(4) (1)	.0359	.0048

Additional Atoms	Distance
C(37) (1)	-1.1472

Mean deviation from plane is .0242 angstroms
Chi-squared: 148.9

Dihedral angles between least-squares planes

plane	plane	angle
3	1	25.38
3	2	157.56

---------- Plane number 4 ----------

Atoms Defining Plane	Distance	esd
N(2) (1)	.0046	.0038
C(6) (1)	-.0085	.0049
C(7) (1)	.0075	.0052
C(8) (1)	-.0029	.0051
C(9) (1)	-.0028	.0049

Mean deviation from plane is .0053 angstroms
Chi-squared: 6.4

Dihedral angles between least-squares planes

plane	plane	angle
4	1	173.37
4	2	11.16
4	3	155.68

---------- Plane number 5 ----------

Atoms Defining Plane	Distance	esd
N(3) (1)	-.0103	.0042
C(11) (1)	.0181	.0056
C(12) (1)	-.0179	.0069
C(13) (1)	.0033	.0066
C(14) (1)	.0098	.0057

Mean deviation from plane is .0119 angstroms
Chi-squared: 22.9

Dihedral angles between least-squares planes

plane	plane	angle
5	1	168.24
5	2	7.13
5	3	164.28
5	4	14.49

---------- Plane number 6 ----------

Atoms Defining Plane	Distance	esd
N(4) (1)	-.0008	.0040
C(16) (1)	-.0006	.0057
C(17) (1)	.0031	.0062
C(18) (1)	-.0033	.0055
C(19) (1)	.0023	.0049

Mean deviation from plane is .0020 angstroms
Chi-squared: .7

Dihedral angles between least-squares planes

plane	plane	angle
6	1	172.23
6	2	3.60
6	3	161.14
6	4	11.19
6	5	4.00

---------- Plane number 7 ----------

Atoms Defining Plane	Distance	esd
N(5) (1)	-.0173	.0038
C(39) (1)	.0232	.0050
C(40) (1)	-.0098	.0055
C(41) (1)	-.0120	.0055
C(42) (1)	.0219	.0048

Additional Atoms	Distance
C(38) (1)	-.8355

Mean deviation from plane is .0168 angstroms
Chi-squared: 62.8

Dihedral angles between least-squares planes

plane	plane	angle
7	1	137.36
7	2	37.39
7	3	156.23
7	4	44.63
7	5	30.91
7	6	34.88

---------- Plane number 8 ----------

Atoms Defining Plane	Distance	esd
N(6) (1)	-.0103	.0038
C(44) (1)	.0121	.0046
C(45) (1)	-.0061	.0050
C(46) (1)	-.0042	.0051
C(47) (1)	.0127	.0048

Mean deviation from plane is .0091 angstroms
Chi-squared: 20.8

Dihedral angles between least-squares planes

plane	plane	angle
8	1	168.63
8	2	6.66
8	3	154.21
8	4	17.56
8	5	10.33
8	6	8.96
8	7	36.13

---------- Plane number 9 ----------

Atoms Defining Plane	Distance	esd
N(7) (1)	.0092	.0039
C(49) (1)	-.0116	.0051
C(50) (1)	.0046	.0057
C(51) (1)	.0059	.0058
C(52) (1)	-.0111	.0049

Mean deviation from plane is .0085 angstroms
Chi-squared: 15.2

Dihedral angles between least-squares planes

plane	plane	angle
9	1	174.86
9	2	1.58
9	3	158.40
9	4	9.83
9	5	6.82
9	6	2.88
9	7	37.56
9	8	8.22

---------- Plane number 10 ----------

Atoms Defining Plane			Distance	esd
N(8)	(	1)	-.0163	.0038
C(54)	(	1)	.0206	.0048
C(55)	(	1)	-.0112	.0054
C(56)	(	1)	-.0076	.0053
C(57)	(	1)	.0203	.0048

Mean deviation from plane is .0152 angstroms
Chi-squared: 53.3

Dihedral angles between least-squares planes

plane	plane	angle
10	1	167.64
10	2	11.16
10	3	166.59
10	4	11.06
10	5	7.67
10	6	7.92
10	7	34.09
10	8	16.82
10	9	9.81

---------- Plane number 11 ----------

Atoms Defining Plane			Distance	esd
N(1)	(	1)	.3427	.0037
N(2)	(	1)	-.0265	.0038
N(3)	(	1)	-.2135	.0042
N(4)	(	1)	.0287	.0040
C(1)	(	1)	-.0384	.0046
C(2)	(	1)	-.4229	.0048
C(3)	(	1)	-.3599	.0052
C(4)	(	1)	.0528	.0048
C(5)	(	1)	.1162	.0052
C(6)	(	1)	.1335	.0049
C(7)	(	1)	.2540	.0052
C(8)	(	1)	.1307	.0051
C(9)	(	1)	-.0424	.0049
C(10)	(	1)	-.1884	.0052
C(11)	(	1)	-.2014	.0056
C(12)	(	1)	-.0804	.0069
C(13)	(	1)	.0555	.0065
C(14)	(	1)	-.0275	.0057
C(15)	(	1)	.0697	.0061
C(16)	(	1)	.1059	.0057
C(17)	(	1)	.1884	.0062
C(18)	(	1)	.1519	.0055
C(19)	(	1)	.0595	.0049
C(20)	(	1)	-.0700	.0048

Additional Atoms			Distance
N(5)	(	1)	4.0114
N(6)	(	1)	4.0764
N(7)	(	1)	4.2756
N(8)	(	1)	4.4539

Mean deviation from plane is .1400 angstroms
Chi-squared: 39166.5

Dihedral angles between least-squares planes

plane	plane	angle
11	1	174.05
11	2	5.43
11	3	160.57
11	4	7.46
11	5	7.06
11	6	3.87
11	7	37.67
11	8	11.97
11	9	3.86
11	10	6.57

---------- Plane number 12 ----------

Atoms Defining Plane			Distance	esd
N(5)	(	1)	-.4272	.0038
N(6)	(	1)	-.0385	.0038
N(7)	(	1)	.1263	.0039
N(8)	(	1)	-.0063	.0038
C(39)	(	1)	.1093	.0050
C(40)	(	1)	.7874	.0053
C(41)	(	1)	.7308	.0054
C(42)	(	1)	.0157	.0047
C(43)	(	1)	-.0687	.0047
C(44)	(	1)	-.1679	.0046
C(45)	(	1)	-.3317	.0050

C(46) (1)	-.2687	.0051
C(47) (1)	-.0677	.0048
C(48) (1)	.0860	.0049
C(49) (1)	.1848	.0051
C(50) (1)	.2919	.0057
C(51) (1)	.2667	.0058
C(52) (1)	.1434	.0050
C(53) (1)	.0007	.0050
C(54) (1)	-.1237	.0049
C(55) (1)	-.3747	.0054
C(56) (1)	-.3503	.0054
C(57) (1)	-.0920	.0049
C(58) (1)	.0644	.0048

Additional Atoms	Distance
N(1) (1)	-3.9777
N(2) (1)	-4.2174
N(3) (1)	-4.6778
N(4) (1)	-4.5658

Mean deviation from plane is .2135 angstroms
Chi-squared: 93559.6

Dihedral angles between least-squares planes

plane	plane	angle
12	1	170.58
12	2	4.10
12	3	161.03
12	4	13.46
12	5	3.27
12	6	2.34
12	7	33.36
12	8	7.44
12	9	4.28
12	10	9.50
12	11	6.21

Distances are in angstroms.

Figure I. An ORTEP drawing of (**15b**)•CH_2Cl_2