

Supporting Information for:

Neutral and Cationic Palladium(II) Bis-pyrazolyl-methane Complexes

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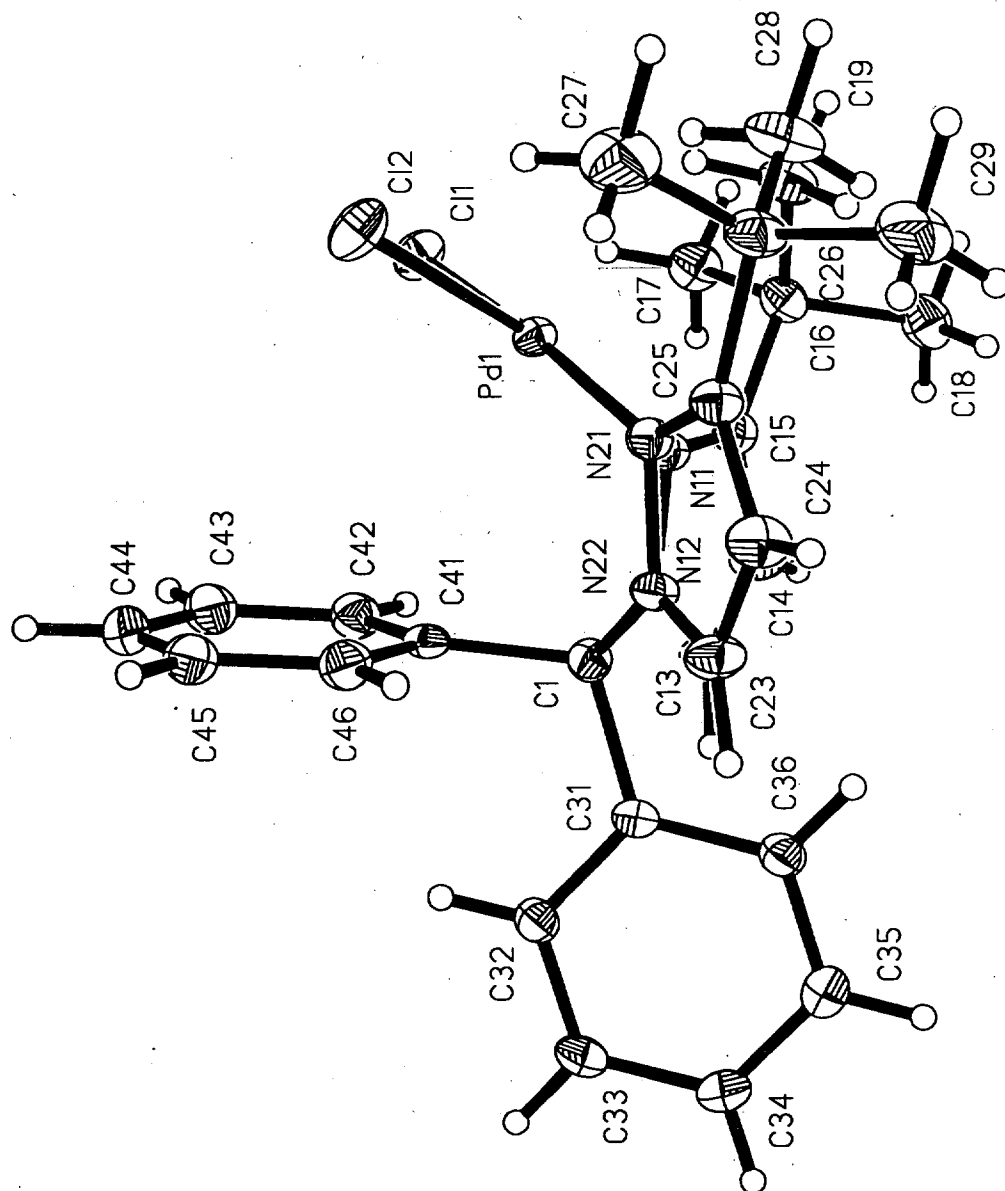
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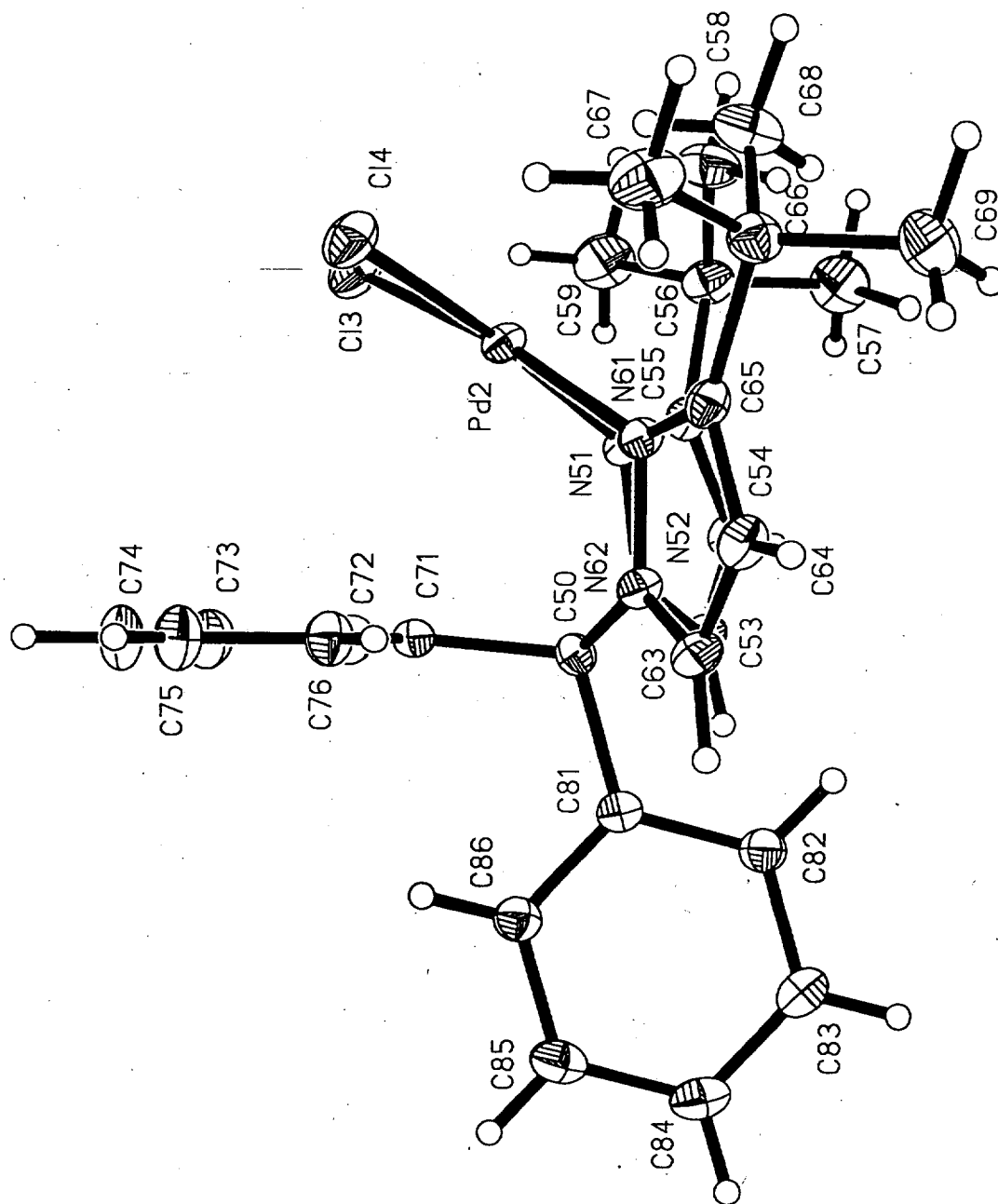
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Table I-1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{C}_{15}\text{H}_{15}\text{Cl}_2\text{U}(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	9770(1)	7895(1)	538(1)	23(1)
Cl(1)	10813(1)	8409(1)	1237(1)	35(1)
Cl(2)	10442(1)	7272(1)	-33(1)	42(1)
C(1)	8776(1)	6713(2)	1005(1)	25(1)
N(11)	9168(1)	8285(1)	1101(1)	24(1)
N(12)	8867(1)	7586(1)	1319(1)	24(1)
C(13)	8646(2)	7842(2)	1817(1)	34(1)
C(14)	8793(2)	8710(2)	1912(1)	36(1)
C(15)	9110(1)	8977(2)	1449(1)	26(1)
C(16)	9309(2)	9913(2)	1340(1)	30(1)
C(17)	10001(2)	10163(2)	1867(1)	38(1)
C(18)	8689(2)	10504(2)	1392(2)	43(1)
C(19)	9396(2)	10050(2)	681(1)	39(1)
N(21)	8810(1)	7388(1)	-9(1)	24(1)
N(22)	8473(1)	6847(1)	310(1)	24(1)
C(23)	7916(2)	6440(2)	-108(1)	32(1)
C(24)	7870(2)	6745(2)	-699(1)	34(1)
C(25)	8426(1)	7348(2)	-625(1)	26(1)
C(26)	8552(2)	7931(2)	-1139(1)	34(1)
C(27)	9049(2)	7482(3)	-1461(2)	56(1)
C(28)	8852(2)	8818(2)	-870(2)	48(1)
C(29)	7823(2)	8092(3)	-1642(2)	58(1)
C(31)	8227(1)	6227(2)	1259(1)	24(1)
C(32)	8442(2)	5542(2)	1683(1)	27(1)
C(33)	7972(2)	5189(2)	1983(1)	30(1)
C(34)	7285(2)	5519(2)	1854(1)	31(1)
C(35)	7059(2)	6193(2)	1422(1)	33(1)
C(36)	7525(1)	6551(2)	1127(1)	29(1)
C(41)	9489(1)	6222(2)	1139(1)	26(1)
C(42)	10066(2)	6407(2)	1666(1)	33(1)
C(43)	10689(2)	5907(2)	1795(2)	41(1)
C(44)	10730(2)	5215(2)	1412(2)	46(1)
C(45)	10157(2)	5020(2)	887(2)	42(1)
C(46)	9535(2)	5520(2)	750(1)	34(1)
Pd(2)	4343(1)	7354(1)	5591(1)	23(1)
Cl(3)	4829(1)	5979(1)	5732(1)	38(1)
Cl(4)	5408(1)	7884(1)	5504(1)	38(1)
C(50)	2975(1)	7648(2)	4516(1)	22(1)
N(51)	3349(1)	6926(1)	5574(1)	24(1)
N(52)	2814(1)	7118(1)	5024(1)	23(1)
C(53)	2191(1)	6735(2)	5033(1)	29(1)
C(54)	2321(2)	6308(2)	5598(1)	33(1)
C(55)	3044(1)	6445(2)	5936(1)	27(1)
C(56)	3416(2)	6150(2)	6615(1)	34(1)
C(57)	2855(2)	6188(2)	6978(2)	51(1)
C(58)	4050(2)	6728(2)	6956(1)	46(1)
C(59)	3661(2)	5194(2)	6608(2)	53(1)
N(61)	3831(1)	8534(1)	5360(1)	23(1)
N(62)	3274(1)	8501(1)	4802(1)	23(1)
C(63)	3109(1)	9316(2)	4569(1)	28(1)

C(64)	29(1)	20(1)	36(2)	4(1)	11(1)	1(1)
C(65)	20(1)	22(1)	32(1)	0(1)	9(1)	-1(1)
C(66)	33(2)	27(2)	32(2)	-3(1)	6(1)	-2(1)
C(67)	35(2)	41(2)	56(2)	-3(2)	4(2)	-13(2)
C(68)	53(2)	43(2)	30(2)	-3(1)	1(2)	-7(2)
C(69)	53(2)	41(2)	55(2)	-21(2)	9(2)	1(2)
C(71)	24(1)	30(2)	21(1)	-1(1)	4(1)	5(1)
C(72)	35(2)	29(2)	39(2)	-2(1)	9(1)	1(1)
C(73)	51(2)	38(2)	54(2)	-10(2)	15(2)	14(2)
C(74)	49(2)	67(3)	54(2)	-12(2)	25(2)	16(2)
C(75)	39(2)	62(2)	49(2)	-1(2)	25(2)	2(2)
C(76)	32(2)	35(2)	37(2)	-1(1)	15(1)	-1(1)
C(81)	23(1)	23(1)	25(1)	2(1)	5(1)	-1(1)
C(82)	28(1)	31(2)	27(1)	1(1)	7(1)	0(1)
C(83)	26(2)	30(2)	42(2)	5(1)	8(1)	3(1)
C(84)	30(2)	33(2)	34(2)	4(1)	-4(1)	-2(1)
C(85)	41(2)	34(2)	26(1)	-1(1)	2(1)	-2(1)
C(86)	31(2)	29(2)	27(1)	1(1)	7(1)	0(1)
C(91)	79(3)	37(2)	56(2)	4(2)	23(2)	0(2)
Cl(5)	79(1)	65(1)	54(1)	-5(1)	31(1)	14(1)
Cl(6)	64(1)	70(1)	55(1)	-7(1)	13(1)	1(1)
Cl(7)	111(2)	72(2)	62(1)	-7(1)	10(1)	-7(1)
Cl(8)	59(2)	83(2)	105(4)	-19(2)	-5(2)	8(2)
C(92)	108(6)	70(5)	62(4)	-6(4)	-28(4)	23(5)
Cl(9)	79(4)	125(9)	143(11)	39(8)	18(5)	7(5)
Cl(10)	46(4)	99(7)	82(7)	-11(5)	-3(3)	-28(5)
C(93)	103(13)	55(11)	79(11)	29(9)	-37(10)	35(10)
Cl(11)	70(2)	50(2)	103(3)	4(2)	11(2)	4(1)
Cl(12)	91(4)	86(3)	90(3)	-10(2)	51(3)	13(2)
C(94)	47(5)	45(5)	70(6)	12(5)	32(4)	6(4)
Cl(13)	82(5)	71(3)	117(7)	-4(4)	-8(5)	-9(3)
Cl(14)	53(3)	58(3)	100(5)	-3(3)	28(3)	-1(2)
C(95)	68(9)	50(8)	61(7)	26(7)	25(7)	9(8)





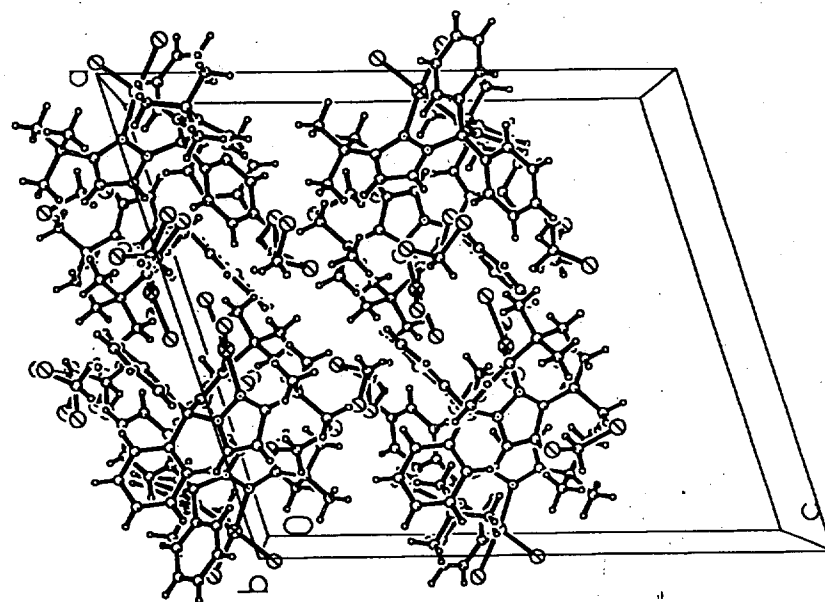
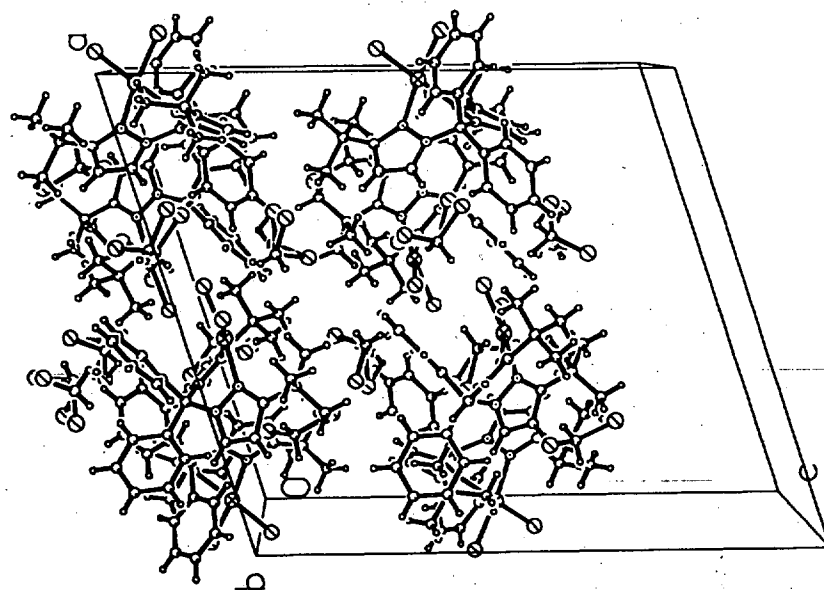


Table I-2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.1.5 CH_2Cl_2 .

The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Pd(1)	21(1)	26(1)	21(1)	0(1)	6(1)	-3(1)
Cl(1)	24(1)	46(1)	32(1)	-4(1)	4(1)	-7(1)
Cl(2)	35(1)	55(1)	41(1)	-12(1)	20(1)	-2(1)
C(1)	26(1)	25(1)	23(1)	1(1)	6(1)	-4(1)
N(11)	24(1)	24(1)	23(1)	2(1)	6(1)	-3(1)
N(12)	26(1)	22(1)	24(1)	1(1)	8(1)	-5(1)
C(13)	42(2)	39(2)	24(1)	-2(1)	16(1)	-10(1)
C(14)	49(2)	33(2)	33(2)	-8(1)	21(1)	-7(1)
C(15)	25(1)	28(1)	24(1)	-1(1)	4(1)	-4(1)
C(16)	36(2)	24(1)	29(1)	-2(1)	7(1)	-2(1)
C(17)	40(2)	30(2)	41(2)	-7(1)	8(1)	-10(1)
C(18)	50(2)	30(2)	46(2)	-2(1)	11(2)	4(2)
C(19)	53(2)	28(2)	36(2)	1(1)	15(2)	-6(1)
N(21)	24(1)	24(1)	23(1)	2(1)	6(1)	-3(1)
N(22)	26(1)	24(1)	22(1)	4(1)	7(1)	-5(1)
C(23)	32(2)	32(2)	30(1)	-1(1)	7(1)	-13(1)
C(24)	36(2)	40(2)	23(1)	0(1)	2(1)	-11(1)
C(25)	29(1)	28(1)	20(1)	-1(1)	7(1)	-4(1)
C(26)	39(2)	39(2)	22(1)	5(1)	7(1)	-7(1)
C(27)	72(3)	67(2)	37(2)	4(2)	29(2)	2(2)
C(28)	69(2)	40(2)	35(2)	8(1)	13(2)	-16(2)
C(29)	50(2)	72(3)	40(2)	26(2)	-5(2)	-11(2)
C(31)	28(1)	22(1)	22(1)	0(1)	8(1)	-4(1)
C(32)	28(1)	24(1)	28(1)	2(1)	7(1)	1(1)
C(33)	38(2)	27(2)	26(1)	6(1)	9(1)	-2(1)
C(34)	33(2)	33(2)	32(2)	-1(1)	15(1)	-8(1)
C(35)	27(1)	36(2)	35(2)	-2(1)	9(1)	1(1)
C(36)	28(1)	27(2)	29(1)	6(1)	5(1)	-1(1)
C(41)	28(1)	26(1)	26(1)	6(1)	12(1)	-3(1)
C(42)	32(2)	34(2)	31(2)	5(1)	8(1)	-1(1)
C(43)	31(2)	47(2)	41(2)	15(2)	5(1)	1(1)
C(44)	36(2)	45(2)	61(2)	22(2)	22(2)	12(2)
C(45)	50(2)	31(2)	56(2)	3(2)	32(2)	4(2)
C(46)	34(2)	33(2)	36(2)	0(1)	14(1)	-2(1)
Pd(2)	19(1)	21(1)	28(1)	2(1)	4(1)	1(1)
Cl(3)	34(1)	26(1)	52(1)	5(1)	9(1)	9(1)
Cl(4)	23(1)	38(1)	52(1)	-3(1)	11(1)	-4(1)
C(50)	24(1)	22(1)	22(1)	0(1)	9(1)	-1(1)
N(51)	21(1)	24(1)	25(1)	3(1)	5(1)	2(1)
N(52)	21(1)	24(1)	23(1)	2(1)	3(1)	-2(1)
C(53)	21(1)	32(2)	34(2)	1(1)	8(1)	-5(1)
C(54)	30(2)	33(2)	37(2)	6(1)	13(1)	-6(1)
C(55)	28(1)	24(1)	29(1)	3(1)	10(1)	1(1)
C(56)	36(2)	33(2)	31(2)	11(1)	8(1)	2(1)
C(57)	59(2)	56(2)	41(2)	20(2)	21(2)	3(2)
C(58)	47(2)	56(2)	28(2)	8(2)	2(1)	-5(2)
C(59)	64(2)	42(2)	49(2)	18(2)	11(2)	14(2)
N(61)	21(1)	22(1)	24(1)	0(1)	4(1)	1(1)
N(62)	21(1)	21(1)	24(1)	1(1)	4(1)	0(1)
C(63)	24(1)	26(1)	31(1)	6(1)	6(1)	3(1)

C(64)	3544(1)	9884(2)	4985(1)	28(1)
C(65)	3979(1)	9385(2)	5485(1)	24(1)
C(66)	4496(2)	9747(2)	6095(1)	32(1)
C(67)	5168(2)	10110(2)	5956(2)	46(1)
C(68)	4699(2)	9072(2)	6625(1)	45(1)
C(69)	4108(2)	10509(2)	6315(2)	51(1)
C(71)	3516(1)	7165(2)	4255(1)	26(1)
C(72)	3485(2)	6258(2)	4198(1)	35(1)
C(73)	3925(2)	5830(2)	3906(2)	48(1)
C(74)	4391(2)	6300(3)	3670(2)	55(1)
C(75)	4418(2)	7198(2)	3721(2)	47(1)
C(76)	3979(2)	7631(2)	4012(1)	34(1)
C(81)	2268(1)	7832(2)	3988(1)	24(1)
C(82)	1689(1)	8232(2)	4125(1)	29(1)
C(83)	1050(2)	8386(2)	3651(1)	33(1)
C(84)	987(2)	8172(2)	3028(1)	35(1)
C(85)	1558(2)	7792(2)	2884(1)	36(1)
C(86)	2194(2)	7618(2)	3358(1)	29(1)
C(91)	2162(2)	6530(2)	1226(2)	57(1)
Cl(5)	2157(1)	5637(1)	733(1)	64(1)
Cl(6)	2598(1)	6274(1)	2029(1)	64(1)
Cl(7)	3068(3)	10903(2)	-2415(1)	85(1)
Cl(8)	3975(3)	12345(3)	-2552(5)	89(2)
C(92)	3638(4)	11746(5)	-2024(3)	92(3)
Cl(9)	2933(5)	11179(13)	-2232(12)	119(5)
Cl(10)	3964(8)	12430(12)	-2426(13)	81(4)
C(93)	3840(5)	11486(12)	-2017(12)	93(8)
Cl(11)	7013(3)	8943(4)	601(5)	78(2)
Cl(12)	6431(7)	8098(6)	-621(5)	84(2)
C(94)	6250(4)	8798(12)	-56(6)	51(3)
Cl(13)	7148(11)	8992(7)	390(13)	99(4)
Cl(14)	6299(7)	8142(8)	-766(8)	69(2)
C(95)	6292(8)	8881(19)	-158(11)	58(6)

Table I-3. Bond lengths [Å] and angles [deg] for 1-1.5 CH₂Cl₂.

Pd(1)-N(11)	2.039(2)
Pd(1)-N(21)	2.050(2)
Pd(1)-Cl(2)	2.2815(8)
Pd(1)-Cl(1)	2.2878(8)
C(1)-N(22)	1.484(3)
C(1)-N(12)	1.489(3)
C(1)-C(41)	1.528(4)
C(1)-C(31)	1.540(4)
N(11)-C(15)	1.332(3)
N(11)-N(12)	1.374(3)
N(12)-C(13)	1.352(3)
C(13)-C(14)	1.360(4)
C(13)-H(13)	0.93
C(14)-C(15)	1.405(4)
C(14)-H(14)	0.93
C(15)-C(16)	1.520(4)
C(16)-C(19)	1.528(4)
C(16)-C(17)	1.539(4)
C(16)-C(18)	1.541(4)
C(17)-H(17A)	0.96
C(17)-H(17B)	0.96
C(17)-H(17C)	0.96
C(18)-H(18A)	0.96
C(18)-H(18B)	0.96
C(18)-H(18C)	0.96
C(19)-H(19A)	0.96
C(19)-H(19B)	0.96
C(19)-H(19C)	0.96
N(21)-C(25)	1.342(3)
N(21)-N(22)	1.372(3)
N(22)-C(23)	1.345(3)
C(23)-C(24)	1.364(4)
C(23)-H(23)	0.93
C(24)-C(25)	1.395(4)
C(24)-H(24)	0.93
C(25)-C(26)	1.521(4)
C(26)-C(28)	1.524(4)
C(26)-C(27)	1.524(5)
C(26)-C(29)	1.536(4)
C(27)-H(27A)	0.96
C(27)-H(27B)	0.96
C(27)-H(27C)	0.96
C(28)-H(28A)	0.96
C(28)-H(28B)	0.96
C(28)-H(28C)	0.96
C(29)-H(29A)	0.96
C(29)-H(29B)	0.96
C(29)-H(29C)	0.96
C(31)-C(32)	1.383(4)
C(31)-C(36)	1.401(4)
C(32)-C(33)	1.391(4)
C(32)-H(32)	0.93
C(33)-C(34)	1.378(4)
C(33)-H(33)	0.93
C(34)-C(35)	1.383(4)
C(34)-H(34)	0.93

C(35)-C(36)	1.380(4)
C(35)-H(35)	0.93
C(36)-H(36)	0.93
C(41)-C(42)	1.383(4)
C(41)-C(46)	1.395(4)
C(42)-C(43)	1.388(4)
C(42)-H(42)	0.93
C(43)-C(44)	1.373(5)
C(43)-H(43)	0.93
C(44)-C(45)	1.378(5)
C(44)-H(44)	0.93
C(45)-C(46)	1.387(4)
C(45)-H(45)	0.93
C(46)-H(46)	0.93
Pd(2)-N(51)	2.034(2)
Pd(2)-N(61)	2.051(2)
Pd(2)-Cl(3)	2.2871(8)
Pd(2)-Cl(4)	2.2909(8)
C(50)-N(62)	1.488(3)
C(50)-N(52)	1.492(3)
C(50)-C(71)	1.535(4)
C(50)-C(81)	1.539(3)
N(51)-C(55)	1.348(3)
N(51)-N(52)	1.374(3)
N(52)-C(53)	1.353(3)
C(53)-C(54)	1.360(4)
C(53)-H(53)	0.93
C(54)-C(55)	1.397(4)
C(54)-H(54)	0.93
C(55)-C(56)	1.523(4)
C(56)-C(58)	1.522(4)
C(56)-C(59)	1.538(4)
C(56)-C(57)	1.539(4)
C(57)-H(57A)	0.96
C(57)-H(57B)	0.96
C(57)-H(57C)	0.96
C(58)-H(58A)	0.96
C(58)-H(58B)	0.96
C(58)-H(58C)	0.96
C(59)-H(59A)	0.96
C(59)-H(59B)	0.96
C(59)-H(59C)	0.96
N(61)-C(65)	1.342(3)
N(61)-N(62)	1.375(3)
N(62)-C(63)	1.349(3)
C(63)-C(64)	1.359(4)
C(63)-H(63)	0.93
C(64)-C(65)	1.398(4)
C(64)-H(64)	0.93
C(65)-C(66)	1.523(4)
C(66)-C(68)	1.520(4)
C(66)-C(67)	1.536(4)
C(66)-C(69)	1.544(4)
C(67)-H(67A)	0.96
C(67)-H(67B)	0.96
C(67)-H(67C)	0.96
C(68)-H(68A)	0.96
C(68)-H(68B)	0.96
C(68)-H(68C)	0.96
C(69)-H(69A)	0.96

C(69)-H(69B)	0.96
C(69)-H(69C)	0.96
C(71)-C(76)	1.379(4)
C(71)-C(72)	1.392(4)
C(72)-C(73)	1.384(4)
C(72)-H(72)	0.93
C(73)-C(74)	1.376(5)
C(73)-H(73)	0.93
C(74)-C(75)	1.377(5)
C(74)-H(74)	0.93
C(75)-C(76)	1.383(4)
C(75)-H(75)	0.93
C(76)-H(76)	0.93
C(81)-C(86)	1.393(4)
C(81)-C(82)	1.394(4)
C(82)-C(83)	1.384(4)
C(82)-H(82)	0.93
C(83)-C(84)	1.382(4)
C(83)-H(83)	0.93
C(84)-C(85)	1.375(4)
C(84)-H(84)	0.93
C(85)-C(86)	1.385(4)
C(85)-H(85)	0.93
C(86)-H(86)	0.93
C(91)-Cl(5)	1.744(4)
C(91)-Cl(6)	1.765(4)
C(91)-H(91A)	0.97
C(91)-H(91B)	0.97
Cl(7)-C(92)	1.75
Cl(8)-C(92)	1.76
C(92)-H(92A)	0.97
C(92)-H(92B)	0.97
C(92)-H(93C)	1.52(2)
C(92)-H(93D)	1.08(2)
Cl(9)-C(93)	1.75
Cl(10)-C(93)	1.76
C(93)-H(93C)	0.97
C(93)-H(93D)	0.97
Cl(11)-C(94)	1.75
Cl(12)-C(94)	1.76
C(94)-H(94A)	0.97
C(94)-H(94B)	0.97
C(94)-H(95A)	1.17(6)
C(94)-H(95B)	0.72(4)
Cl(13)-C(95)	1.75
Cl(14)-C(95)	1.76
C(95)-H(95A)	0.97
C(95)-H(95B)	0.97

N(11)-Pd(1)-N(21)	83.01(8)
N(11)-Pd(1)-Cl(2)	172.06(6)
N(21)-Pd(1)-Cl(2)	95.20(7)
N(11)-Pd(1)-Cl(1)	92.69(6)
N(21)-Pd(1)-Cl(1)	174.18(6)
Cl(2)-Pd(1)-Cl(1)	88.52(3)
N(22)-C(1)-N(12)	108.2(2)
N(22)-C(1)-C(41)	108.8(2)
N(12)-C(1)-C(41)	112.1(2)
N(22)-C(1)-C(31)	109.9(2)
N(12)-C(1)-C(31)	105.1(2)

C(41)-C(1)-C(31)	112.6(2)
C(15)-N(11)-N(12)	107.2(2)
C(15)-N(11)-Pd(1)	138.4(2)
N(12)-N(11)-Pd(1)	111.9(2)
C(13)-N(12)-N(11)	109.5(2)
C(13)-N(12)-C(1)	127.9(2)
N(11)-N(12)-C(1)	122.4(2)
N(12)-C(13)-C(14)	107.7(2)
N(12)-C(13)-H(13)	126.2(2)
C(14)-C(13)-H(13)	126.2(2)
C(13)-C(14)-C(15)	106.8(3)
C(13)-C(14)-H(14)	126.6(2)
C(15)-C(14)-H(14)	126.6(2)
N(11)-C(15)-C(14)	108.7(2)
N(11)-C(15)-C(16)	125.9(2)
C(14)-C(15)-C(16)	125.3(2)
C(15)-C(16)-C(19)	112.7(2)
C(15)-C(16)-C(17)	108.8(2)
C(19)-C(16)-C(17)	111.3(2)
C(15)-C(16)-C(18)	107.2(2)
C(19)-C(16)-C(18)	107.7(2)
C(17)-C(16)-C(18)	109.0(2)
C(16)-C(17)-H(17A)	109.5(2)
C(16)-C(17)-H(17B)	109.5(2)
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5(2)
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5(2)
C(16)-C(18)-H(18B)	109.5(2)
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5(2)
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5(2)
C(16)-C(19)-H(19B)	109.5(2)
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5(2)
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(25)-N(21)-N(22)	106.6(2)
C(25)-N(21)-Pd(1)	138.2(2)
N(22)-N(21)-Pd(1)	114.72(15)
C(23)-N(22)-N(21)	109.8(2)
C(23)-N(22)-C(1)	129.1(2)
N(21)-N(22)-C(1)	120.7(2)
N(22)-C(23)-C(24)	107.7(2)
N(22)-C(23)-H(23)	126.13(15)
C(24)-C(23)-H(23)	126.1(2)
C(23)-C(24)-C(25)	106.8(2)
C(23)-C(24)-H(24)	126.6(2)
C(25)-C(24)-H(24)	126.6(2)
N(21)-C(25)-C(24)	108.9(2)
N(21)-C(25)-C(26)	124.3(2)
C(24)-C(25)-C(26)	126.5(2)
C(25)-C(26)-C(28)	111.1(2)
C(25)-C(26)-C(27)	110.6(3)
C(28)-C(26)-C(27)	111.0(3)
C(25)-C(26)-C(29)	108.0(2)
C(28)-C(26)-C(29)	107.6(3)

C(27)-C(26)-C(29)	108.4(3)
C(26)-C(27)-H(27A)	109.5(2)
C(26)-C(27)-H(27B)	109.5(2)
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5(2)
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5(2)
C(26)-C(28)-H(28B)	109.5(2)
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5(2)
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(26)-C(29)-H(29A)	109.5(2)
C(26)-C(29)-H(29B)	109.5(2)
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5(2)
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(32)-C(31)-C(36)	119.0(2)
C(32)-C(31)-C(1)	120.7(2)
C(36)-C(31)-C(1)	119.7(2)
C(31)-C(32)-C(33)	120.5(3)
C(31)-C(32)-H(32)	119.7(2)
C(33)-C(32)-H(32)	119.7(2)
C(34)-C(33)-C(32)	120.0(3)
C(34)-C(33)-H(33)	120.0(2)
C(32)-C(33)-H(33)	120.0(2)
C(33)-C(34)-C(35)	120.1(3)
C(33)-C(34)-H(34)	119.9(2)
C(35)-C(34)-H(34)	119.9(2)
C(36)-C(35)-C(34)	120.2(3)
C(36)-C(35)-H(35)	119.9(2)
C(34)-C(35)-H(35)	119.9(2)
C(35)-C(36)-C(31)	120.1(2)
C(35)-C(36)-H(36)	119.9(2)
C(31)-C(36)-H(36)	119.93(15)
C(42)-C(41)-C(46)	119.2(3)
C(42)-C(41)-C(1)	121.6(2)
C(46)-C(41)-C(1)	118.9(2)
C(41)-C(42)-C(43)	120.0(3)
C(41)-C(42)-H(42)	120.0(2)
C(43)-C(42)-H(42)	120.0(2)
C(44)-C(43)-C(42)	120.5(3)
C(44)-C(43)-H(43)	119.8(2)
C(42)-C(43)-H(43)	119.8(2)
C(43)-C(44)-C(45)	120.1(3)
C(43)-C(44)-H(44)	120.0(2)
C(45)-C(44)-H(44)	120.0(2)
C(44)-C(45)-C(46)	119.9(3)
C(44)-C(45)-H(45)	120.0(2)
C(46)-C(45)-H(45)	120.0(2)
C(45)-C(46)-C(41)	120.3(3)
C(45)-C(46)-H(46)	119.9(2)
C(41)-C(46)-H(46)	119.9(2)
N(51)-Pd(2)-N(61)	83.62(8)
N(51)-Pd(2)-Cl(3)	93.43(6)
N(61)-Pd(2)-Cl(3)	173.02(6)
N(51)-Pd(2)-Cl(4)	174.00(6)
N(61)-Pd(2)-Cl(4)	93.05(6)

Cl(3) - Pd(2) - Cl(4)	89.32(3)
N(62) - C(50) - N(52)	107.4(2)
N(62) - C(50) - C(71)	110.8(2)
N(52) - C(50) - C(71)	110.2(2)
N(62) - C(50) - C(81)	108.0(2)
N(52) - C(50) - C(81)	109.0(2)
C(71) - C(50) - C(81)	111.3(2)
C(55) - N(51) - N(52)	106.7(2)
C(55) - N(51) - Pd(2)	138.8(2)
N(52) - N(51) - Pd(2)	114.4(2)
C(53) - N(52) - N(51)	109.8(2)
C(53) - N(52) - C(50)	129.8(2)
N(51) - N(52) - C(50)	120.3(2)
N(52) - C(53) - C(54)	107.6(2)
N(52) - C(53) - H(53)	126.22(15)
C(54) - C(53) - H(53)	126.2(2)
C(53) - C(54) - C(55)	107.3(2)
C(53) - C(54) - H(54)	126.4(2)
C(55) - C(54) - H(54)	126.4(2)
N(51) - C(55) - C(54)	108.6(2)
N(51) - C(55) - C(56)	125.5(2)
C(54) - C(55) - C(56)	125.8(2)
C(58) - C(56) - C(55)	112.9(2)
C(58) - C(56) - C(59)	110.4(3)
C(55) - C(56) - C(59)	109.2(3)
C(58) - C(56) - C(57)	108.5(3)
C(55) - C(56) - C(57)	107.5(2)
C(59) - C(56) - C(57)	108.2(3)
C(56) - C(57) - H(57A)	109.5(2)
C(56) - C(57) - H(57B)	109.5(2)
H(57A) - C(57) - H(57B)	109.5
C(56) - C(57) - H(57C)	109.5(2)
H(57A) - C(57) - H(57C)	109.5
H(57B) - C(57) - H(57C)	109.5
C(56) - C(58) - H(58A)	109.5(2)
C(56) - C(58) - H(58B)	109.5(2)
H(58A) - C(58) - H(58B)	109.5
C(56) - C(58) - H(58C)	109.5(2)
H(58A) - C(58) - H(58C)	109.5
H(58B) - C(58) - H(58C)	109.5
C(56) - C(59) - H(59A)	109.5(2)
C(56) - C(59) - H(59B)	109.5(2)
H(59A) - C(59) - H(59B)	109.5
C(56) - C(59) - H(59C)	109.5(2)
H(59A) - C(59) - H(59C)	109.5
H(59B) - C(59) - H(59C)	109.5
C(65) - N(61) - N(62)	106.5(2)
C(65) - N(61) - Pd(2)	137.9(2)
N(62) - N(61) - Pd(2)	112.6(2)
C(63) - N(62) - N(61)	109.9(2)
C(63) - N(62) - C(50)	129.0(2)
N(61) - N(62) - C(50)	121.0(2)
N(62) - C(63) - C(64)	107.7(2)
N(62) - C(63) - H(63)	126.15(15)
C(64) - C(63) - H(63)	126.2(2)
C(63) - C(64) - C(65)	106.9(2)
C(63) - C(64) - H(64)	126.5(2)
C(65) - C(64) - H(64)	126.5(2)
N(61) - C(65) - C(64)	108.9(2)
N(61) - C(65) - C(66)	125.3(2)

C(64)-C(65)-C(66)	125.6(2)
C(68)-C(66)-C(65)	112.5(2)
C(68)-C(66)-C(67)	111.0(3)
C(65)-C(66)-C(67)	109.3(2)
C(68)-C(66)-C(69)	108.0(3)
C(65)-C(66)-C(69)	107.3(2)
C(67)-C(66)-C(69)	108.6(3)
C(66)-C(67)-H(67A)	109.5(2)
C(66)-C(67)-H(67B)	109.5(2)
H(67A)-C(67)-H(67B)	109.5
C(66)-C(67)-H(67C)	109.5(2)
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(66)-C(68)-H(68A)	109.5(2)
C(66)-C(68)-H(68B)	109.5(2)
H(68A)-C(68)-H(68B)	109.5
C(66)-C(68)-H(68C)	109.5(2)
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(66)-C(69)-H(69A)	109.5(2)
C(66)-C(69)-H(69B)	109.5(2)
H(69A)-C(69)-H(69B)	109.5
C(66)-C(69)-H(69C)	109.5(2)
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
C(76)-C(71)-C(72)	119.7(3)
C(76)-C(71)-C(50)	120.2(2)
C(72)-C(71)-C(50)	119.8(3)
C(73)-C(72)-C(71)	119.7(3)
C(73)-C(72)-H(72)	120.1(2)
C(71)-C(72)-H(72)	120.1(2)
C(74)-C(73)-C(72)	120.2(3)
C(74)-C(73)-H(73)	119.9(2)
C(72)-C(73)-H(73)	119.9(2)
C(73)-C(74)-C(75)	120.2(3)
C(73)-C(74)-H(74)	119.9(2)
C(75)-C(74)-H(74)	119.9(2)
C(74)-C(75)-C(76)	120.0(3)
C(74)-C(75)-H(75)	120.0(2)
C(76)-C(75)-H(75)	120.0(2)
C(71)-C(76)-C(75)	120.2(3)
C(71)-C(76)-H(76)	119.9(2)
C(75)-C(76)-H(76)	119.9(2)
C(86)-C(81)-C(82)	118.3(2)
C(86)-C(81)-C(50)	120.8(2)
C(82)-C(81)-C(50)	120.9(2)
C(83)-C(82)-C(81)	120.8(3)
C(83)-C(82)-H(82)	119.6(2)
C(81)-C(82)-H(82)	119.60(15)
C(84)-C(83)-C(82)	120.1(3)
C(84)-C(83)-H(83)	119.9(2)
C(82)-C(83)-H(83)	119.9(2)
C(85)-C(84)-C(83)	119.6(3)
C(85)-C(84)-H(84)	120.2(2)
C(83)-C(84)-H(84)	120.2(2)
C(84)-C(85)-C(86)	120.6(3)
C(84)-C(85)-H(85)	119.7(2)
C(86)-C(85)-H(85)	119.7(2)
C(85)-C(86)-C(81)	120.5(3)
C(85)-C(86)-H(86)	119.8(2)

C(81)-C(86)-H(86)	119.8(2)
Cl(5)-C(91)-Cl(6)	111.3(2)
Cl(5)-C(91)-H(91A)	109.36(15)
Cl(6)-C(91)-H(91A)	109.36(14)
Cl(5)-C(91)-H(91B)	109.36(13)
Cl(6)-C(91)-H(91B)	109.36(13)
H(91A)-C(91)-H(91B)	108.0
Cl(7)-C(92)-Cl(8)	111.4
Cl(7)-C(92)-H(92A)	109.3
Cl(8)-C(92)-H(92A)	109.4
Cl(7)-C(92)-H(92B)	109.3
Cl(8)-C(92)-H(92B)	109.4
H(92A)-C(92)-H(92B)	107.9
H(93C)-C(92)-H(93D)	72.2(10)
Cl(9)-C(93)-Cl(10)	111.4
H(92A)-C(93)-H(92B)	83(3)
Cl(9)-C(93)-H(93C)	109.3
Cl(10)-C(93)-H(93C)	109.4
Cl(9)-C(93)-H(93D)	109.3
Cl(10)-C(93)-H(93D)	109.3
H(93C)-C(93)-H(93D)	108.0
Cl(11)-C(94)-Cl(12)	111.4
Cl(11)-C(94)-H(94A)	109.3
Cl(12)-C(94)-H(94A)	109.4
Cl(11)-C(94)-H(94B)	109.3
Cl(12)-C(94)-H(94B)	109.4
H(94A)-C(94)-H(94B)	108.0
H(95A)-C(94)-H(95B)	111(4)
Cl(13)-C(95)-Cl(14)	111.4
H(94A)-C(95)-H(94B)	98(3)
Cl(13)-C(95)-H(95A)	109.3
Cl(14)-C(95)-H(95A)	109.4
Cl(13)-C(95)-H(95B)	109.4
Cl(14)-C(95)-H(95B)	109.4
H(95A)-C(95)-H(95B)	108.0

Symmetry transformations used to generate equivalent atoms:

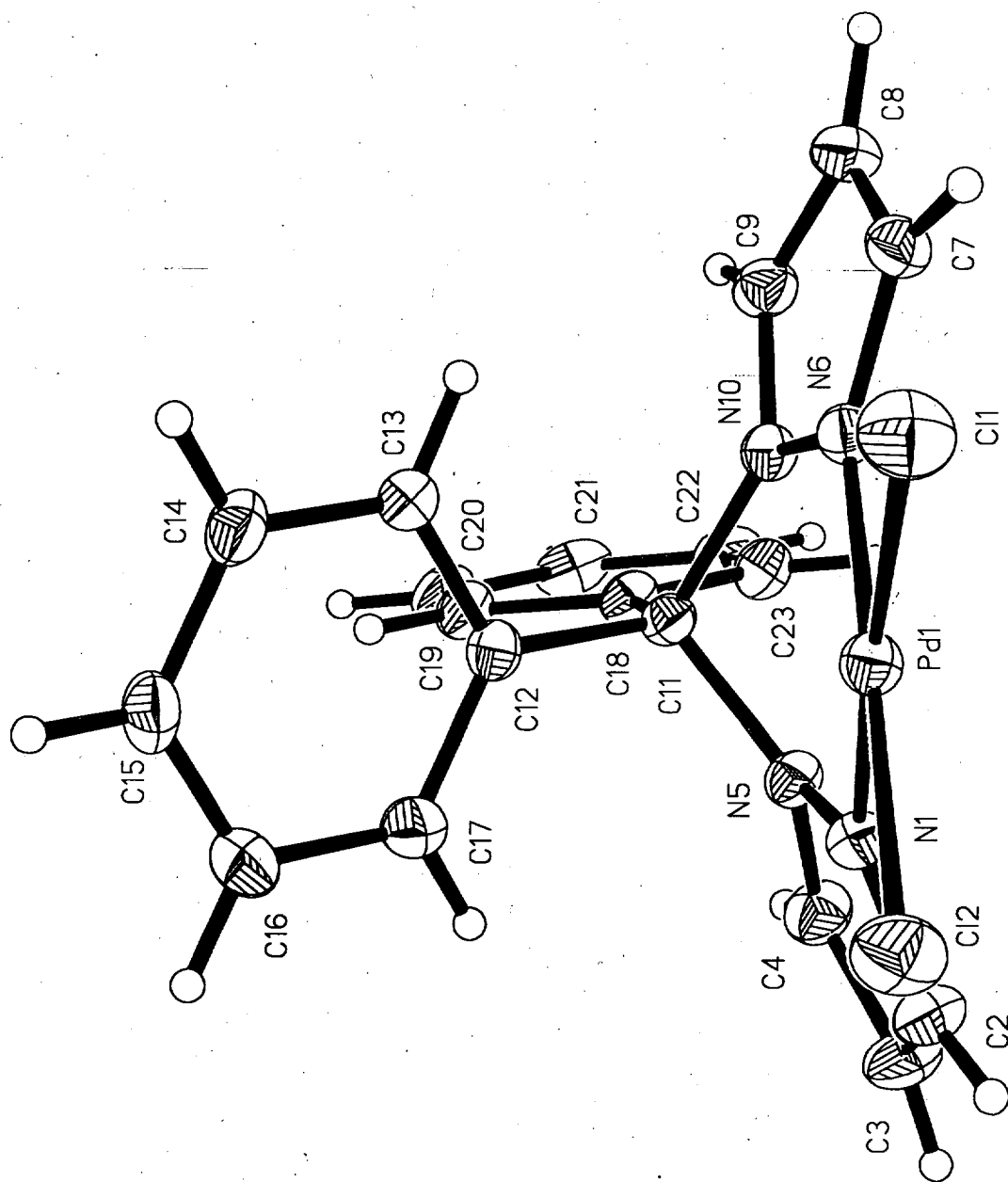
Table I-4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.1.5 CH_2Cl_2 .

	x	y	z	U(eq)
H(13)	8432(2)	7488(2)	2051(1)	41
H(14)	8702(2)	9059(2)	2224(1)	43
H(17A)	10113(7)	10766(4)	1821(6)	57
H(17B)	10391(3)	9802(10)	1835(6)	57
H(17C)	9930(4)	10078(14)	2275(2)	57
H(18A)	8801(6)	11103(2)	1332(11)	65
H(18B)	8628(8)	10436(11)	1805(4)	65
H(18C)	8253(3)	10341(10)	1073(7)	65
H(19A)	9480(12)	10659(3)	623(4)	58
H(19B)	8965(5)	9866(13)	363(1)	58
H(19C)	9796(7)	9712(11)	644(4)	58
H(23)	7617(2)	6026(2)	-10(1)	39
H(24)	7532(2)	6582(2)	-1079(1)	41
H(27A)	8850(8)	6925(8)	-1624(11)	84
H(27B)	9514(5)	7399(16)	-1157(4)	84
H(27C)	9095(12)	7840(9)	-1804(8)	84
H(28A)	9321(6)	8741(3)	-570(9)	72
H(28B)	8537(7)	9080(7)	-661(10)	72
H(28C)	8887(12)	9191(6)	-1209(2)	72
H(29A)	7630(7)	7545(4)	-1833(9)	87
H(29B)	7887(3)	8479(15)	-1963(7)	87
H(29C)	7497(5)	8351(17)	-1444(3)	87
H(32)	8904(2)	5315(2)	1769(1)	32
H(33)	8121(2)	4731(2)	2270(1)	36
H(34)	6972(2)	5288(2)	2059(1)	38
H(35)	6592(2)	6407(2)	1330(1)	39
H(36)	7372(1)	7008(2)	839(1)	35
H(42)	10038(2)	6865(2)	1935(1)	39
H(43)	11081(2)	6043(2)	2144(2)	49
H(44)	11146(2)	4877(2)	1506(2)	55
H(45)	10186(2)	4553(2)	626(2)	51
H(46)	9147(2)	5386(2)	397(1)	40
H(53)	1754(1)	6759(2)	4713(1)	35
H(54)	1990(2)	5986(2)	5733(1)	39
H(57A)	3083(3)	6052(17)	7417(3)	76
H(57B)	2480(7)	5771(12)	6800(8)	76
H(57C)	2653(10)	6765(5)	6944(10)	76
H(58A)	4243(8)	6537(10)	7389(3)	69
H(58B)	3892(3)	7324(3)	6948(10)	69
H(58C)	4415(6)	6687(12)	6747(7)	69
H(59A)	3841(13)	4982(6)	7036(2)	80
H(59B)	4034(10)	5162(3)	6408(11)	80
H(59C)	3260(4)	4841(4)	6375(10)	80
H(63)	2760(1)	9462(2)	4192(1)	33
H(64)	3551(1)	10489(2)	4945(1)	34
H(67A)	5482(6)	10369(14)	6335(3)	69
H(67B)	5027(2)	10545(11)	5628(8)	69
H(67C)	5414(7)	9642(3)	5819(11)	69
H(68A)	4999(10)	9340(4)	7007(3)	67
H(68B)	4955(11)	8600(8)	6505(5)	67
H(68C)	4270(2)	8850(11)	6699(8)	67

H(69A)	4421 (5)	10757 (11)	6699 (7)	77
H(69B)	3679 (7)	10295 (4)	6393 (12)	77
H(69C)	3982 (12)	10950 (8)	5991 (5)	77
H(72)	3169 (2)	5940 (2)	4356 (1)	42
H(73)	3907 (2)	5224 (2)	3869 (2)	58
H(74)	4687 (2)	6010 (3)	3475 (2)	66
H(75)	4732 (2)	7514 (2)	3560 (2)	57
H(76)	3997 (2)	8237 (2)	4044 (1)	41
H(82)	1733 (1)	8397 (2)	4541 (1)	35
H(83)	663 (2)	8634 (2)	3752 (1)	40
H(84)	561 (2)	8284 (2)	2708 (1)	42
H(85)	1517 (2)	7650 (2)	2465 (1)	43
H(86)	2575 (2)	7356 (2)	3255 (1)	35
H(91A)	1671 (2)	6708 (2)	1178 (2)	68
H(91B)	2407 (2)	7017 (2)	1099 (2)	68
H(92A)	4037 (6)	11499 (9)	-1690 (4)	110
H(92B)	3375 (9)	12137 (6)	-1826 (7)	110
H(93C)	4122 (12)	11009 (13)	-2110 (29)	111
H(93D)	4011 (20)	11595 (29)	-1562 (11)	111
H(94A)	6092 (13)	9362 (14)	-250 (7)	61
H(94B)	5864 (4)	8552 (23)	84 (9)	61
H(95A)	6126 (20)	9449 (20)	-343 (17)	70
H(95B)	5957 (12)	8675 (39)	60 (15)	70

Table II-1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{C}_{20}\text{H}_{12}\text{Cl}_2\text{Pd}$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pd(1)	5584(1)	1388(1)	3341(1)	26(1)
Cl(1)	6303(1)	2624(1)	2952(1)	44(1)
Cl(2)	6598(1)	1322(1)	4213(1)	44(1)
N(1)	4986(1)	264(1)	3653(1)	29(1)
C(2)	5349(2)	-394(2)	4003(1)	37(1)
C(3)	4720(2)	-1081(2)	4055(2)	42(1)
C(4)	3952(2)	-816(2)	3712(1)	36(1)
N(5)	4126(1)	-3(1)	3457(1)	26(1)
N(6)	4673(1)	1444(1)	2576(1)	27(1)
C(7)	4729(2)	1864(2)	1996(1)	33(1)
C(8)	3914(2)	1760(2)	1631(1)	37(1)
C(9)	3351(2)	1245(2)	2019(1)	32(1)
N(10)	3823(1)	1040(1)	2581(1)	25(1)
C(11)	3447(2)	656(2)	3207(1)	25(1)
C(12)	3343(2)	1381(1)	3736(1)	26(1)
C(13)	3262(2)	2253(2)	3546(1)	32(1)
C(14)	3188(2)	2906(2)	4028(1)	37(1)
C(15)	3171(2)	2696(2)	4698(1)	38(1)
C(16)	3226(2)	1816(2)	4887(1)	40(1)
C(17)	3323(2)	1166(2)	4410(1)	34(1)
C(18)	2544(2)	179(2)	3037(1)	28(1)
C(19)	1719(2)	378(2)	3359(1)	32(1)
C(20)	913(2)	-79(2)	3204(1)	38(1)
C(21)	922(2)	-728(2)	2722(2)	41(1)
C(22)	1742(2)	-926(2)	2394(1)	39(1)
C(23)	2549(2)	-479(2)	2550(1)	33(1)
C(31)	856(3)	1388(2)	5533(2)	63(1)
Cl(3)	426(1)	1411(1)	4723(1)	80(1)
Cl(4)	1488(1)	430(1)	5711(1)	78(1)



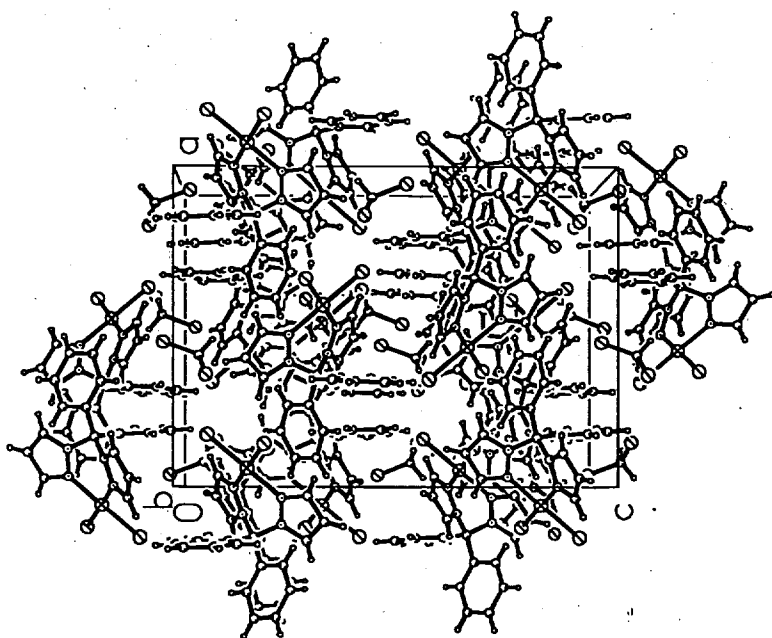
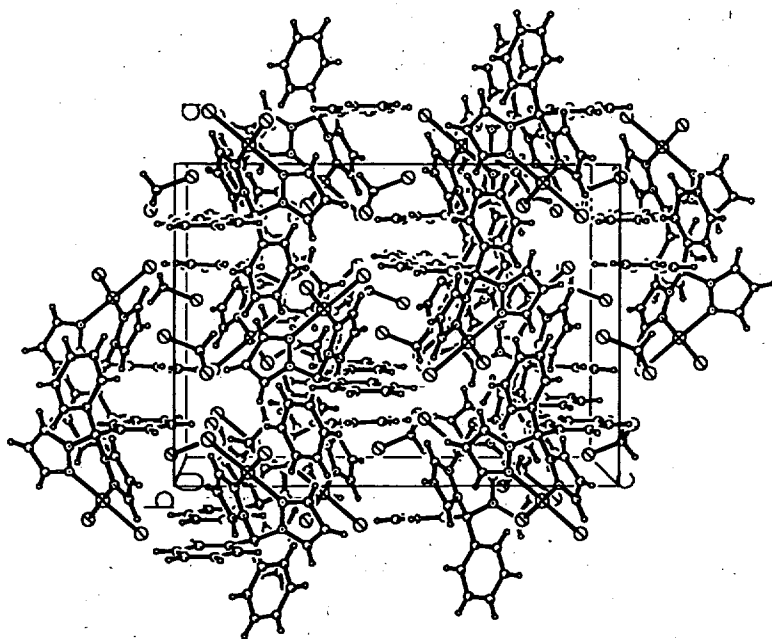


Table II-2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2-CH₂Cl₂.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Pd(1)	24(1)	27(1)	27(1)	0(1)	1(1)	-1(1)
Cl(1)	42(1)	39(1)	51(1)	6(1)	1(1)	-14(1)
Cl(2)	37(1)	56(1)	40(1)	1(1)	-11(1)	-7(1)
N(1)	28(1)	30(1)	28(1)	2(1)	-2(1)	2(1)
C(2)	36(1)	37(1)	37(1)	6(1)	-6(1)	8(1)
C(3)	47(2)	31(1)	48(2)	14(1)	-4(1)	4(1)
C(4)	39(1)	26(1)	44(2)	5(1)	2(1)	0(1)
N(5)	27(1)	23(1)	30(1)	1(1)	0(1)	1(1)
N(6)	27(1)	26(1)	27(1)	1(1)	2(1)	1(1)
C(7)	38(1)	30(1)	30(1)	4(1)	7(1)	0(1)
C(8)	46(2)	39(1)	26(1)	6(1)	-1(1)	5(1)
C(9)	36(1)	32(1)	29(1)	-1(1)	-6(1)	4(1)
N(10)	27(1)	24(1)	25(1)	-1(1)	0(1)	1(1)
C(11)	26(1)	23(1)	27(1)	2(1)	1(1)	3(1)
C(12)	22(1)	26(1)	29(1)	-2(1)	1(1)	0(1)
C(13)	36(1)	30(1)	29(1)	2(1)	2(1)	6(1)
C(14)	39(1)	26(1)	45(2)	-3(1)	5(1)	6(1)
C(15)	36(1)	40(1)	38(1)	-14(1)	0(1)	7(1)
C(16)	46(2)	48(2)	27(1)	-3(1)	-1(1)	7(1)
C(17)	40(1)	32(1)	31(1)	3(1)	0(1)	2(1)
C(18)	27(1)	23(1)	34(1)	3(1)	-2(1)	1(1)
C(19)	32(1)	26(1)	39(1)	2(1)	1(1)	2(1)
C(20)	27(1)	35(1)	52(2)	10(1)	1(1)	2(1)
C(21)	35(1)	33(1)	55(2)	11(1)	-14(1)	-7(1)
C(22)	46(2)	28(1)	42(2)	-1(1)	-12(1)	-2(1)
C(23)	34(1)	28(1)	37(1)	-2(1)	-1(1)	2(1)
C(31)	76(2)	65(2)	49(2)	-2(2)	-2(2)	5(2)
Cl(3)	83(1)	105(1)	51(1)	-16(1)	-14(1)	36(1)
Cl(4)	93(1)	57(1)	84(1)	24(1)	-16(1)	-5(1)

Table II-3. Bond lengths [Å] and angles [deg] for 2·CH₂Cl₂.

Pd(1)-N(1)	2.018(2)
Pd(1)-N(6)	2.020(2)
Pd(1)-Cl(2)	2.2787(7)
Pd(1)-Cl(1)	2.2876(7)
N(1)-C(2)	1.330(3)
N(1)-N(5)	1.363(3)
C(2)-C(3)	1.390(4)
C(2)-H(2)	0.93
C(3)-C(4)	1.364(4)
C(3)-H(3)	0.93
C(4)-N(5)	1.363(3)
C(4)-H(4)	0.93
N(5)-C(11)	1.492(3)
N(6)-C(7)	1.328(3)
N(6)-N(10)	1.372(3)
C(7)-C(8)	1.394(4)
C(7)-H(7)	0.93
C(8)-C(9)	1.370(4)
C(8)-H(8)	0.93
C(9)-N(10)	1.351(3)
C(9)-H(9)	0.93
N(10)-C(11)	1.485(3)
C(11)-C(18)	1.530(3)
C(11)-C(12)	1.537(3)
C(12)-C(17)	1.388(3)
C(12)-C(13)	1.389(3)
C(13)-C(14)	1.390(3)
C(13)-H(13)	0.93
C(14)-C(15)	1.377(4)
C(14)-H(14)	0.93
C(15)-C(16)	1.396(4)
C(15)-H(15)	0.93
C(16)-C(17)	1.382(4)
C(16)-H(16)	0.93
C(17)-H(17)	0.93
C(18)-C(19)	1.386(3)
C(18)-C(23)	1.399(3)
C(19)-C(20)	1.391(4)
C(19)-H(19)	0.93
C(20)-C(21)	1.382(4)
C(20)-H(20)	0.93
C(21)-C(22)	1.385(4)
C(21)-H(21)	0.93
C(22)-C(23)	1.385(4)
C(22)-H(22)	0.93
C(23)-H(23)	0.93
C(31)-Cl(3)	1.736(4)
C(31)-Cl(4)	1.759(4)
C(31)-H(31A)	0.97
C(31)-H(31B)	0.97
N(1)-Pd(1)-N(6)	89.51(8)
N(1)-Pd(1)-Cl(2)	89.99(6)
N(6)-Pd(1)-Cl(2)	179.32(6)
N(1)-Pd(1)-Cl(1)	177.23(6)
N(6)-Pd(1)-Cl(1)	90.14(6)

Cl(2)-Pd(1)-Cl(1)	90.38(3)
C(2)-N(1)-N(5)	106.5(2)
C(2)-N(1)-Pd(1)	129.4(2)
N(5)-N(1)-Pd(1)	123.64(14)
N(1)-C(2)-C(3)	110.5(2)
N(1)-C(2)-H(2)	124.73(15)
C(3)-C(2)-H(2)	124.7(2)
C(4)-C(3)-C(2)	105.6(2)
C(4)-C(3)-H(3)	127.2(2)
C(2)-C(3)-H(3)	127.20(15)
N(5)-C(4)-C(3)	107.9(2)
N(5)-C(4)-H(4)	126.04(14)
C(3)-C(4)-H(4)	126.0(2)
N(1)-N(5)-C(4)	109.4(2)
N(1)-N(5)-C(11)	119.6(2)
C(4)-N(5)-C(11)	128.1(2)
C(7)-N(6)-N(10)	106.1(2)
C(7)-N(6)-Pd(1)	130.0(2)
N(10)-N(6)-Pd(1)	123.91(15)
N(6)-C(7)-C(8)	110.6(2)
N(6)-C(7)-H(7)	124.72(15)
C(8)-C(7)-H(7)	124.72(15)
C(9)-C(8)-C(7)	105.6(2)
C(9)-C(8)-H(8)	127.2(2)
C(7)-C(8)-H(8)	127.21(15)
N(10)-C(9)-C(8)	107.8(2)
N(10)-C(9)-H(9)	126.10(14)
C(8)-C(9)-H(9)	126.1(2)
C(9)-N(10)-N(6)	109.9(2)
C(9)-N(10)-C(11)	127.5(2)
N(6)-N(10)-C(11)	120.6(2)
N(10)-C(11)-N(5)	108.0(2)
N(10)-C(11)-C(18)	108.1(2)
N(5)-C(11)-C(18)	108.3(2)
N(10)-C(11)-C(12)	109.4(2)
N(5)-C(11)-C(12)	108.5(2)
C(18)-C(11)-C(12)	114.3(2)
C(17)-C(12)-C(13)	119.4(2)
C(17)-C(12)-C(11)	120.2(2)
C(13)-C(12)-C(11)	120.5(2)
C(12)-C(13)-C(14)	120.1(2)
C(12)-C(13)-H(13)	119.96(14)
C(14)-C(13)-H(13)	119.96(15)
C(15)-C(14)-C(13)	120.7(2)
C(15)-C(14)-H(14)	119.66(15)
C(13)-C(14)-H(14)	119.66(15)
C(14)-C(15)-C(16)	119.1(2)
C(14)-C(15)-H(15)	120.45(15)
C(16)-C(15)-H(15)	120.45(15)
C(17)-C(16)-C(15)	120.5(2)
C(17)-C(16)-H(16)	119.8(2)
C(15)-C(16)-H(16)	119.77(15)
C(16)-C(17)-C(12)	120.3(2)
C(16)-C(17)-H(17)	119.9(2)
C(12)-C(17)-H(17)	119.87(14)
C(19)-C(18)-C(23)	119.1(2)
C(19)-C(18)-C(11)	121.6(2)
C(23)-C(18)-C(11)	119.4(2)
C(18)-C(19)-C(20)	120.3(2)
C(18)-C(19)-H(19)	119.84(14)

C(20)-C(19)-H(19)	119.8(2)
C(21)-C(20)-C(19)	120.4(3)
C(21)-C(20)-H(20)	119.8(2)
C(19)-C(20)-H(20)	119.8(2)
C(20)-C(21)-C(22)	119.7(2)
C(20)-C(21)-H(21)	120.2(2)
C(22)-C(21)-H(21)	120.2(2)
C(21)-C(22)-C(23)	120.3(2)
C(21)-C(22)-H(22)	119.9(2)
C(23)-C(22)-H(22)	119.9(2)
C(22)-C(23)-C(18)	120.3(2)
C(22)-C(23)-H(23)	119.8(2)
C(18)-C(23)-H(23)	119.85(15)
Cl(3)-C(31)-Cl(4)	113.0(2)
Cl(3)-C(31)-H(31A)	108.99(14)
Cl(4)-C(31)-H(31A)	108.99(13)
Cl(3)-C(31)-H(31B)	108.99(13)
Cl(4)-C(31)-H(31B)	108.99(14)
H(31A)-C(31)-H(31B)	107.8

Symmetry transformations used to generate equivalent atoms:

Table II-4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2-CH₂Cl₂.

	x	y	z	U(eq)
H(2)	5941(2)	-394(2)	4187(1)	44
H(3)	4805(2)	-1611(2)	4277(2)	50
H(4)	3407(2)	-1134(2)	3661(1)	44
H(7)	5241(2)	2184(2)	1854(1)	39
H(8)	3780(2)	1991(2)	1212(1)	44
H(9)	2752(2)	1068(2)	1914(1)	38
H(13)	3258(2)	2401(2)	3095(1)	38
H(14)	3149(2)	3490(2)	3897(1)	44
H(15)	3123(2)	3134(2)	5019(1)	45
H(16)	3198(2)	1667(2)	5337(1)	48
H(17)	3375(2)	583(2)	4542(1)	41
H(19)	1705(2)	818(2)	3681(1)	39
H(20)	364(2)	54(2)	3426(1)	46
H(21)	381(2)	-1031(2)	2618(2)	49
H(22)	1750(2)	-1360(2)	2068(1)	47
H(23)	3098(2)	-617(2)	2329(1)	40
H(31A)	342(3)	1433(2)	5845(2)	76
H(31B)	1253(3)	1894(2)	5601(2)	76

Table III-1. COSY spectrum of **1**

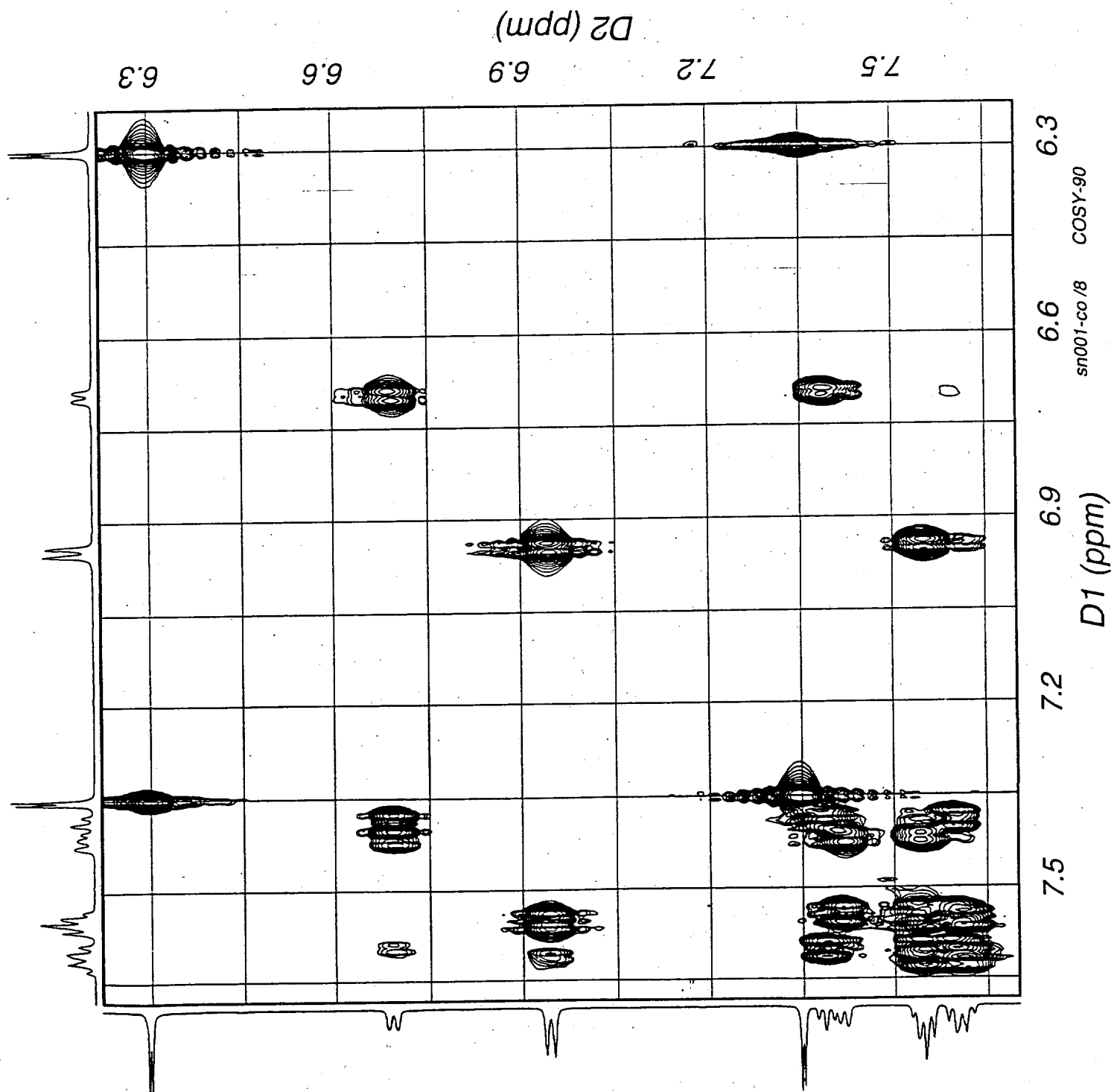


Table III-2. NOESY spectrum of 1

NOESY 1.05 mlx
Current Data Parameters
NAME sn001-no
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date 980113
Time 6.19
PULPROG noesy-hc
SOLVENT CD2Cl2
AQ 0.4260040 sec
FIDRES 1.173753 Hz
DQ 104.0 usrc
RG 512
NUCLEUS 1H
H1 0 dB
D1 4.0000000 sec
P1 6.8 usrc
D0 0.0000030 sec
P0 6.8 usrc
D8 1.0000000 sec
DE 148.5 usrc
SF01 600.1406100 MHz
SM 4907.69 Hz
T0 4096
NS 16
DS 8
IN0 0.0002060 sec

F1 - Acquisition Parameters
N00 1
T0 340
SF01 600.1406 MHz
FIDRES 14.140271 Hz
SN 8.011 ppm

F2 - Processing parameters
SI 1024
SF 600.1376109 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 0.10

F1 - Processing parameters
SI 1024
MC2 1024
SF 600.1376109 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PL0 7.759 ppm
F2L0 4656.48 Hz
F2PH1 6.179 ppm
F2H1 3708.08 Hz
F1PL0 7.751 ppm
F1L0 4651.74 Hz
F1PH1 6.171 ppm
F1H1 3703.35 Hz
F2PPMCM 0.10535 ppm/cm
F2HZCM 63.22615 Hz/cm
F1PPMCM 0.10535 ppm/cm
F1HZCM 63.22615 Hz/cm

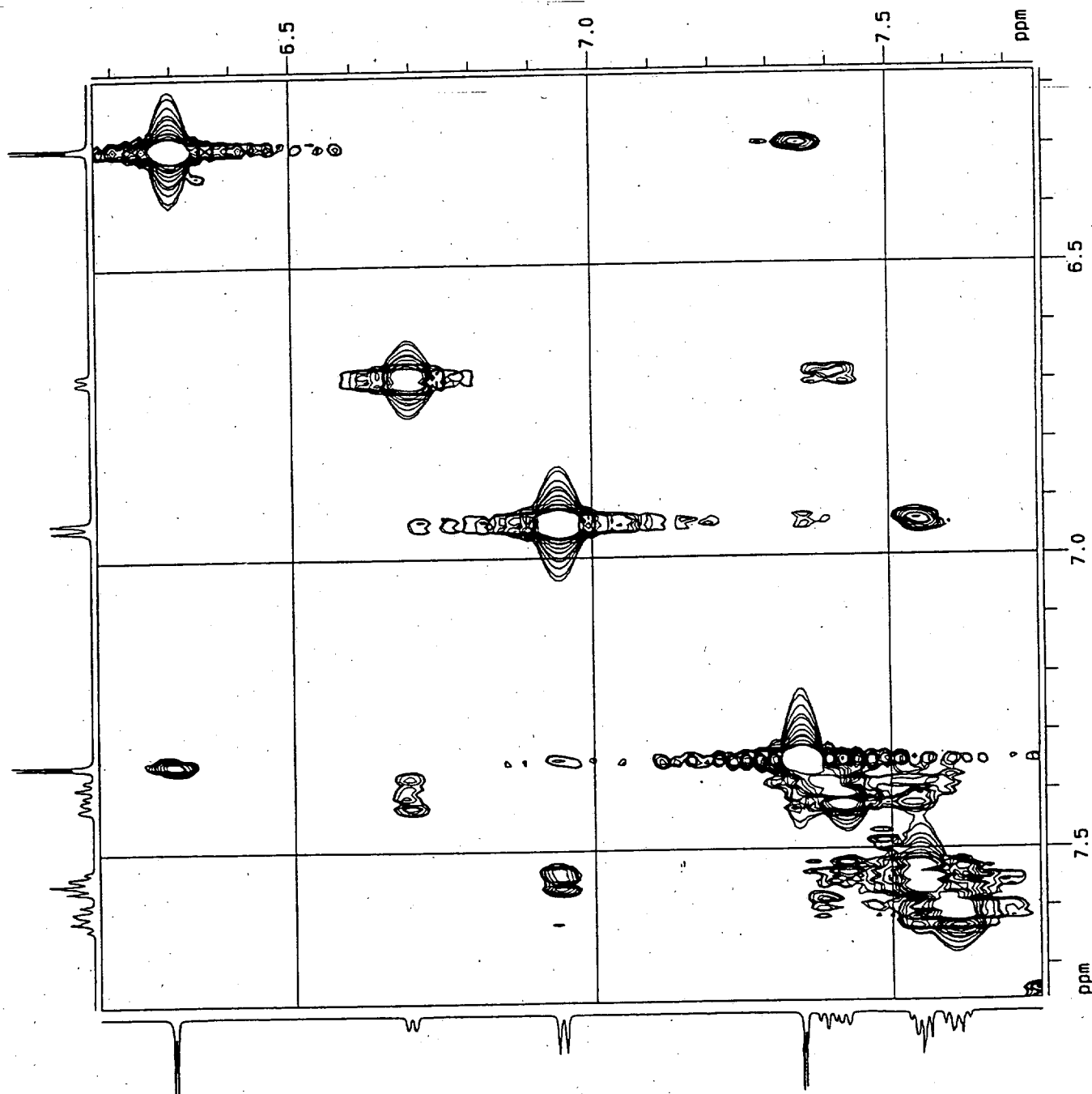


Table IV-1. COSY spectrum of **2**

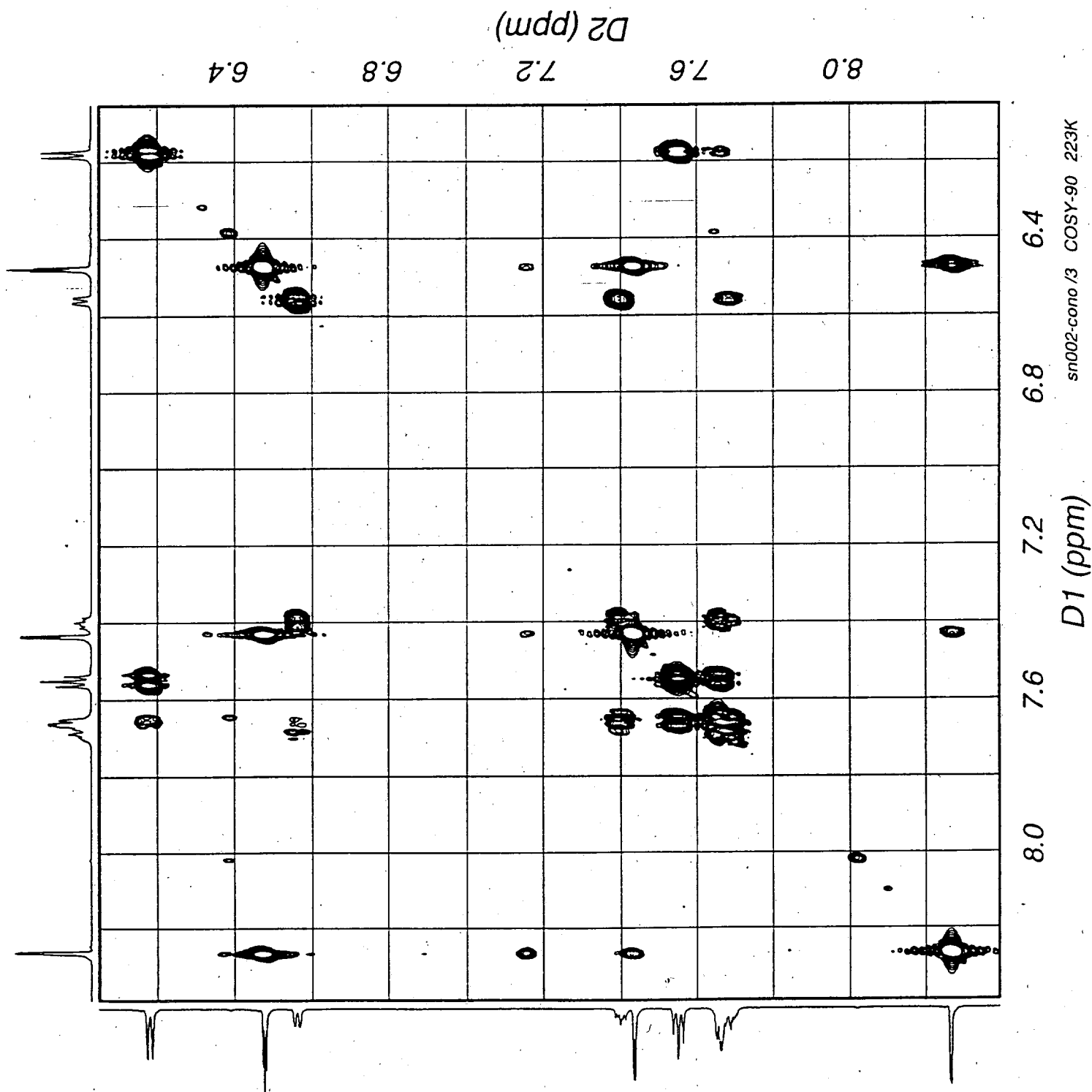


Table IV-2. NOESY spectrum of 2

