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Supporting Information

Synthesis of Chiral (Diaminocarbene)Pd(allyl)Cl Complexes

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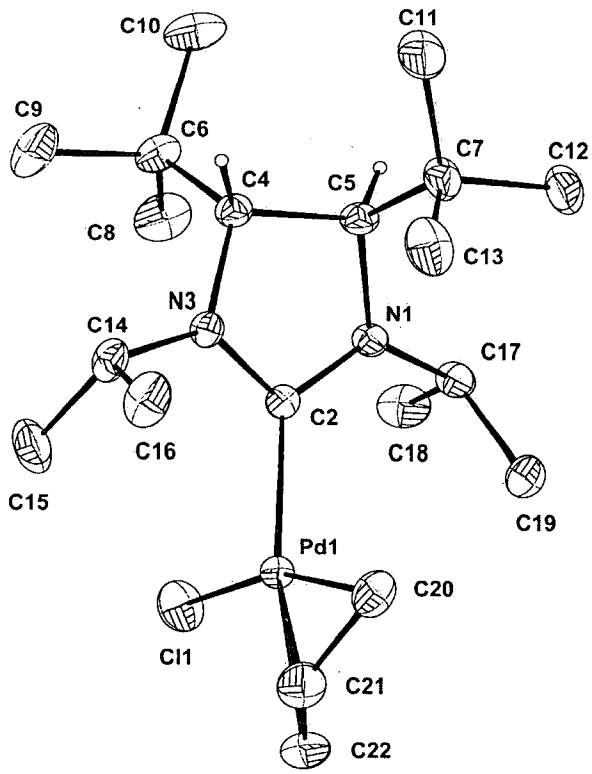
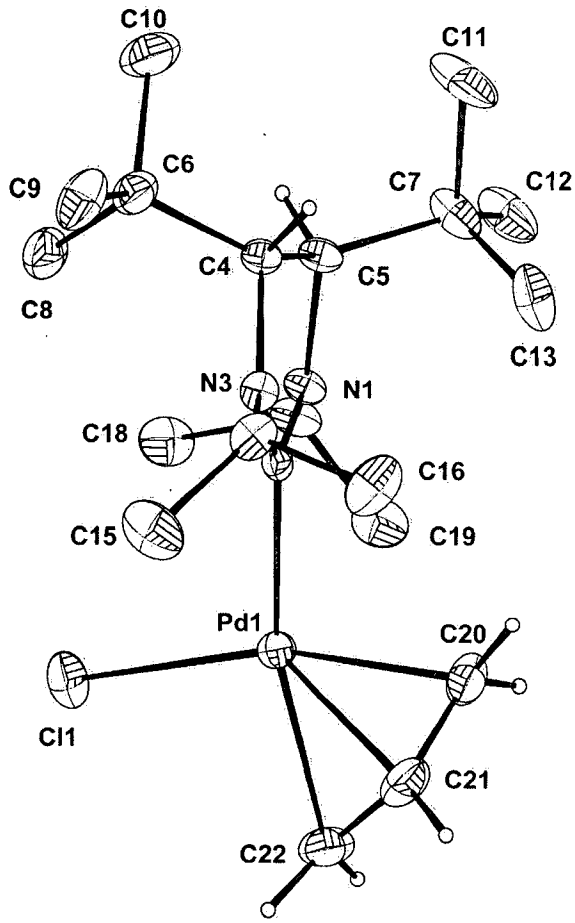
Crystal structure – complex 7a





Crystal structure information – complex 7a

Formula	$C_{20}H_{39}ClN_2Pd$		
Crystal Class	Monoclinic		
Space Group	$P\ 2_1$		
Flack parameter	0.06(3)		
a (Å)	9.0266(12)	alpha	90
b (Å)	9.0113(5)	beta	91.41(1)
c (Å)	13.7577(15)	gamma	90
Volume	1118.7(2)		
Z	2		
Radiation type	Mo Kα		
Wavelength (Å)	0.710730		
Density	1.33		
$M(g.mol^{-1})$	449.40		
$\mu(mm^{-1})$	0.953		
Temperature (K)	295		
Size (mm)	0.20 x 0.21 x 0.45		
Colour	colourless		
Shape	stick		
Diffractometer type	Nonius KAPPACCD		
Reflections measured	7611		
Independent reflections	3678		
Rint	0.05		
Theta min, max	1 26.00		
Hmin, Hmax	-11 11		
Kmin, Kmax	-11 9		
Lmin, Lmax	-16 16		
Refinement	on F		
R-factor	0.0220	$R = \sum \lvert F_0 - F_c \rvert / \sum F_0$	
Weighted R-factor	0.0244	$Rw^* = [\sum w (F_0 - F_c)^2 / \sum w F_0^2]^{1/2}$	
Delta Rho min ($/Å^3$)	-0.47		
Delta Rho max ($/Å^3$)	0.35		
Reflections used	3319		
sigma(I) limit	3.00		
Number of parameters	218		
Goodness of fit	1.080		

Weighting scheme of the form $w=w'[1-((|F_0|-|F_c|)/6\sigma(F_0))^2]^2$ with $w'=1/\sum_r A_r T_r(X)$ with coefficients 0.408, 0.126 and 0.250 for a Chebychev series for which $X=F_c/F_c(max)$

Atom coordinates and Uiso or Ueq:

Atom	x/a	y/b	z/c	U(equiv)
Pd(1)	-0.59166(2)	-0.00439(7)	-0.721626(12)	0.0302
Cl(1)	-0.73709(11)	0.16893(13)	-0.63608(6)	0.0539
N(1)	-0.3773(2)	0.2070(3)	-0.81702(17)	0.0296
C(2)	-0.4065(3)	0.1226(3)	-0.7378(2)	0.0269
N(3)	-0.2896(3)	0.1311(3)	-0.67757(17)	0.0300
C(4)	-0.1760(3)	0.2370(4)	-0.7083(2)	0.0316
C(5)	-0.2227(3)	0.2626(4)	-0.8155(2)	0.0334
C(6)	-0.1674(4)	0.3818(4)	-0.6460(2)	0.0437
C(7)	-0.1242(4)	0.1822(5)	-0.8899(2)	0.0493
C(8)	-0.3163(4)	0.4636(4)	-0.6465(3)	0.0588
C(9)	-0.1220(5)	0.3472(5)	-0.5403(3)	0.0666
C(10)	-0.0459(4)	0.4827(8)	-0.6861(3)	0.0685
C(11)	0.0331(4)	0.2431(7)	-0.8802(3)	0.0784
C(12)	-0.1785(4)	0.2137(6)	-0.9949(2)	0.0621
C(13)	-0.1238(4)	0.0159(7)	-0.8742(3)	0.0652
C(14)	-0.2606(4)	0.0312(4)	-0.5926(2)	0.0384
C(15)	-0.3842(5)	0.0367(5)	-0.5197(2)	0.0663
C(16)	-0.2290(5)	-0.1258(5)	-0.6221(3)	0.0608
C(17)	-0.4881(3)	0.2672(4)	-0.8879(2)	0.0376
C(18)	-0.5897(4)	0.3779(4)	-0.8415(3)	0.0513
C(19)	-0.5736(4)	0.1466(5)	-0.9423(2)	0.0515
C(20)	-0.5235(4)	-0.1905(4)	-0.8038(2)	0.0490
C(21)	-0.6255(5)	-0.2380(4)	-0.7353(3)	0.0537
C(22)	-0.7664(4)	-0.1754(5)	-0.7342(3)	0.0582

Atom	x/a	y/b	z/c	U(iso)
H(41)	-0.0724	0.1991	-0.6993	0.076(2)
H(51)	-0.2122	0.3685	-0.8360	0.076(2)
H(81)	-0.3069	0.5554	-0.6060	0.076(2)
H(82)	-0.3454	0.4911	-0.7147	0.076(2)
H(83)	-0.3937	0.3974	-0.6189	0.076(2)
H(91)	-0.1173	0.4415	-0.5020	0.076(2)
H(92)	-0.0225	0.2983	-0.5383	0.076(2)
H(93)	-0.1967	0.2792	-0.5115	0.076(2)
H(101)	-0.0398	0.5758	-0.6465	0.076(2)
H(102)	-0.0709	0.5082	-0.7553	0.076(2)
H(103)	0.0513	0.4299	-0.6823	0.076(2)
H(111)	0.0975	0.1918	-0.9278	0.076(2)
H(112)	0.0321	0.3520	-0.8936	0.076(2)
H(113)	0.0726	0.2248	-0.8127	0.076(2)
H(121)	-0.1134	0.1608	-1.0413	0.076(2)
H(122)	-0.1746	0.3229	-1.0076	0.076(2)
H(123)	-0.2828	0.1779	-1.0038	0.076(2)
H(131)	-0.0594	-0.0322	-0.9232	0.076(2)
H(132)	-0.2271	-0.0230	-0.8818	0.076(2)
H(133)	-0.0844	-0.0067	-0.8073	0.076(2)
H(141)	-0.1688	0.0705	-0.5597	0.076(2)
H(151)	-0.3598	-0.0317	-0.4642	0.076(2)
H(152)	-0.4793	0.0051	-0.5520	0.076(2)
H(153)	-0.3942	0.1403	-0.4946	0.076(2)
H(161)	-0.2104	-0.1875	-0.5627	0.076(2)
H(162)	-0.3159	-0.1664	-0.6598	0.076(2)

H(163)	-0.1393	-0.1277	-0.6634	0.076(2)
H(171)	-0.4307	0.3218	-0.9379	0.076(2)
H(181)	-0.6626	0.4159	-0.8914	0.076(2)
H(182)	-0.5300	0.4625	-0.8145	0.076(2)
H(183)	-0.6440	0.3286	-0.7879	0.076(2)
H(191)	-0.6465	0.1932	-0.9889	0.076(2)
H(192)	-0.5030	0.0833	-0.9788	0.076(2)
H(193)	-0.6276	0.0839	-0.8947	0.076(2)
H(201)	-0.5538	-0.1948	-0.8741	0.076(2)
H(202)	-0.4184	-0.2245	-0.7957	0.076(2)
H(211)	-0.6185	-0.3430	-0.7122	0.076(2)
H(221)	-0.8292	-0.1789	-0.7950	0.076(2)
H(222)	-0.8294	-0.1944	-0.6768	0.076(2)

Thermal parameters:

Atom	u(11)	u(22)	u(33)	u(23)	u(13)	u(12)
Pd(1)	0.03059(9)	0.0306(1)	0.02940(8)	0.00044(15)	0.00034(5)	-0.00304(17)
Cl(1)	0.0563(5)	0.0546(6)	0.0514(4)	-0.0049(4)	0.0124(4)	0.0134(4)
N(1)	0.020(1)	0.0356(14)	0.0328(11)	0.007(1)	-0.0019(8)	0.003(1)
C(2)	0.0249(13)	0.0262(16)	0.0297(12)	-0.004(1)	0.002(1)	0.0048(11)
N(3)	0.0311(13)	0.0300(14)	0.0285(12)	0.0028(9)	-0.004(1)	0.0040(11)
C(4)	0.0234(13)	0.0355(17)	0.0358(14)	0.0005(11)	-0.001(1)	-0.0013(12)
C(5)	0.0213(13)	0.0405(18)	0.0384(15)	0.0049(12)	-0.0006(11)	-0.0021(13)
C(6)	0.0403(18)	0.0378(18)	0.0529(18)	-0.0076(14)	-0.0047(14)	-0.0058(15)
C(7)	0.0299(15)	0.084(3)	0.0345(15)	0.0044(16)	0.0047(12)	0.0049(18)
C(8)	0.0494(18)	0.043(3)	0.084(2)	-0.0166(18)	0.0010(16)	0.0070(17)
C(9)	0.080(3)	0.059(3)	0.060(2)	-0.0227(19)	-0.018(2)	-0.007(2)
C(10)	0.0544(18)	0.052(3)	0.099(3)	-0.008(3)	-0.0030(17)	-0.020(3)
C(11)	0.0258(16)	0.155(5)	0.055(2)	0.003(3)	0.0068(15)	-0.004(2)
C(12)	0.0402(18)	0.111(4)	0.0352(16)	0.0093(18)	0.0051(14)	0.001(2)
C(13)	0.068(2)	0.072(4)	0.0566(18)	-0.007(2)	0.0174(15)	0.028(3)
C(14)	0.0444(15)	0.036(3)	0.0343(13)	0.0057(12)	-0.0133(11)	0.0016(14)
C(15)	0.066(2)	0.097(5)	0.0352(15)	0.0188(18)	0.0046(14)	-0.000(2)
C(16)	0.086(3)	0.037(2)	0.058(2)	0.0094(18)	-0.021(2)	0.006(2)
C(17)	0.0262(14)	0.047(2)	0.0397(15)	0.0158(13)	-0.0029(11)	0.0013(14)
C(18)	0.0370(17)	0.044(2)	0.072(2)	0.0155(17)	-0.0070(16)	0.0111(16)
C(19)	0.0405(18)	0.073(3)	0.0404(17)	0.0083(17)	-0.0099(14)	-0.0048(18)
C(20)	0.056(2)	0.041(2)	0.0501(19)	-0.0152(15)	-0.0028(15)	0.0016(17)
C(21)	0.070(3)	0.030(2)	0.060(2)	-0.0030(15)	-0.0005(18)	-0.0078(18)
C(22)	0.054(2)	0.059(3)	0.062(2)	-0.0046(18)	0.0027(17)	-0.025(2)

Distances and angles:

Pd(1) - Cl(1)	2.3714(9)	C(5) - C(7)	1.552(4)
Pd(1) - C(2)	2.042(3)	C(6) - C(8)	1.533(5)
Pd(1) - C(20)	2.123(4)	C(6) - C(9)	1.533(5)
Pd(1) - C(21)	2.134(4)	C(6) - C(10)	1.537(6)
Pd(1) - C(22)	2.209(4)	C(7) - C(11)	1.525(5)
N(1) - C(2)	1.360(4)	C(7) - C(12)	1.540(5)
N(1) - C(5)	1.482(4)	C(7) - C(13)	1.515(8)
N(1) - C(17)	1.483(3)	C(14) - C(15)	1.519(5)
C(2) - N(3)	1.328(4)	C(14) - C(16)	1.501(6)
N(3) - C(4)	1.470(4)	C(17) - C(18)	1.508(5)
N(3) - C(14)	1.493(4)	C(17) - C(19)	1.519(5)
C(4) - C(5)	1.541(4)	C(20) - C(21)	1.400(5)
C(4) - C(6)	1.562(4)	C(21) - C(22)	1.392(6)

Cl(1) - Pd(1) - C(2)	98.61(8)	Cl(1) - Pd(1) - C(20)	162.98(11)
C(2) - Pd(1) - C(20)	97.80(13)	Cl(1) - Pd(1) - C(21)	127.85(11)
C(2) - Pd(1) - C(21)	131.18(14)	C(20) - Pd(1) - C(21)	38.41(15)
Cl(1) - Pd(1) - C(22)	95.48(12)	C(2) - Pd(1) - C(22)	165.25(13)
C(20) - Pd(1) - C(22)	67.84(16)	C(21) - Pd(1) - C(22)	37.33(16)
C(2) - N(1) - C(5)	112.3(2)	C(2) - N(1) - C(17)	126.2(2)
C(5) - N(1) - C(17)	120.3(2)	Pd(1) - C(2) - N(1)	125.2(2)
Pd(1) - C(2) - N(3)	127.2(2)	N(1) - C(2) - N(3)	107.5(2)
C(2) - N(3) - C(4)	114.0(2)	C(2) - N(3) - C(14)	125.1(3)
C(4) - N(3) - C(14)	120.4(2)	N(3) - C(4) - C(5)	101.3(2)
N(3) - C(4) - C(6)	114.2(2)	C(5) - C(4) - C(6)	114.1(3)
N(1) - C(5) - C(4)	101.4(2)	N(1) - C(5) - C(7)	112.8(3)
C(4) - C(5) - C(7)	114.4(2)	C(4) - C(6) - C(8)	111.5(3)
C(4) - C(6) - C(9)	111.1(3)	C(8) - C(6) - C(9)	108.4(3)
C(4) - C(6) - C(10)	108.9(3)	C(8) - C(6) - C(10)	110.3(4)
C(9) - C(6) - C(10)	106.5(3)	C(5) - C(7) - C(11)	108.8(3)
C(5) - C(7) - C(12)	111.0(3)	C(11) - C(7) - C(12)	106.9(3)
C(5) - C(7) - C(13)	111.6(3)	C(11) - C(7) - C(13)	110.1(4)
C(12) - C(7) - C(13)	108.4(3)	N(3) - C(14) - C(15)	112.4(3)
N(3) - C(14) - C(16)	112.8(3)	C(15) - C(14) - C(16)	110.9(3)
N(1) - C(17) - C(18)	111.8(3)	N(1) - C(17) - C(19)	112.8(3)
C(18) - C(17) - C(19)	112.0(3)	Pd(1) - C(20) - C(21)	71.2(2)
Pd(1) - C(21) - C(20)	70.3(2)	Pd(1) - C(21) - C(22)	74.2(2)
C(20) - C(21) - C(22)	120.0(4)	Pd(1) - C(22) - C(21)	68.4(2)