

ORGANOMETALLICS

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Table S1 : positional parameters for non hydrogen atoms and their E.S.D.

Atom	x	y	z	Ueqv
PD	0.5	0.5	0.5	0.02876(7)
CL1	0.64396(6)	0.32454(5)	0.53466(5)	0.0500(2)
CL2	0.28434(6)	0.39045(6)	0.54570(5)	0.0564(3)
C1	0.4492(2)	0.0177(2)	0.1933(2)	0.0389(9)
N1	0.5178(2)	-0.0849(1)	0.2312(1)	0.0392(8)
C2	0.5855(2)	-0.0594(2)	0.3342(2)	0.046(1)
C3	0.5580(2)	0.0610(2)	0.3578(2)	0.045(1)
N2	0.4708(2)	0.1080(1)	0.2694(1)	0.0358(7)
C4	0.5227(3)	-0.2053(2)	0.1720(2)	0.056(1)
C5	0.4140(2)	0.2372(2)	0.2593(2)	0.0391(9)
C6	0.5294(2)	0.3239(2)	0.2087(2)	0.044(1)
C7	0.4702(2)	0.4555(2)	0.1917(2)	0.043(1)
C8	0.3474(3)	0.4682(2)	0.1013(2)	0.050(1)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S2 : positional parameters for hydrogen atoms

Atom	x	y	z	Ueqv
H1	0.3938	0.0252	0.1234	0.0507
H2	0.6416	-0.1165	0.3805	0.0605
H3	0.5924	0.1055	0.4232	0.0585
H4	0.4672	-0.1994	0.1021	0.0747
H5	0.6249	-0.2264	0.1574	0.0747
H6	0.4793	-0.2681	0.2181	0.0747
H7	0.3897	0.2668	0.3328	0.0511
H8	0.3255	0.2373	0.2120	0.0511
H9	0.5578	0.2915	0.1371	0.0580
H10	0.6157	0.3271	0.2582	0.0580
H11	0.5526	0.5073	0.1712	0.0574
H12	0.4308	0.4836	0.2617	0.0574
H13	0.3166	0.5532	0.0959	0.0657
H14	0.3850	0.4416	0.0302	0.0657
H15	0.2632	0.4179	0.1207	0.0657

Table S3 : thermal parameters for anisotropic atoms

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
PD	0.0331(1)	0.0277(1)	0.0259(1)	0.0001(1)	-0.0041(1)	-0.0007(1)
CL1	0.0575(3)	0.0361(2)	0.0604(3)	0.0132(2)	-0.0184(2)	-0.0042(2)
CL2	0.0453(2)	0.0622(3)	0.0637(3)	-0.0150(2)	0.0004(2)	0.0138(3)
C1	0.0410(9)	0.0364(9)	0.0393(9)	-0.0009(7)	-0.0030(8)	-0.0013(7)
N1	0.0380(7)	0.0349(7)	0.0454(8)	-0.0008(6)	0.0024(7)	-0.0017(7)
C2	0.043(1)	0.045(1)	0.051(1)	0.0030(9)	-0.0075(9)	0.004(1)
C3	0.049(1)	0.044(1)	0.0415(9)	0.0011(9)	-0.0102(8)	-0.0025(9)
N2	0.0375(7)	0.0327(7)	0.0375(7)	-0.0020(6)	-0.0033(6)	-0.0007(6)
C4	0.060(1)	0.039(1)	0.073(1)	0.003(1)	0.003(1)	-0.016(1)
C5	0.0390(8)	0.0342(8)	0.0447(9)	0.0024(7)	-0.0009(8)	-0.0032(8)
C6	0.0430(9)	0.0387(9)	0.052(1)	0.0016(8)	0.0004(9)	0.0040(9)
C7	0.055(1)	0.0331(8)	0.044(1)	-0.0034(9)	-0.0016(9)	-0.0032(9)
C8	0.055(1)	0.043(1)	0.053(1)	-0.000(1)	-0.003(1)	0.005(1)

Table S4 : bond distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
PD	CL1	2.2974(4)	C2	C3	1.340(3)
PD	CL2	2.3096(5)	C3	N2	1.376(2)
C1	N1	1.325(2)	N2	C5	1.472(2)
C1	N2	1.328(2)	C5	C6	1.510(3)
N1	C2	1.367(2)	C6	C7	1.512(3)
N1	C4	1.465(2)	C7	C8	1.508(3)

Table S5 : bond angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
CL1	PD	CL2	90.05(2)	C2	C3	N2	107.2(1)
CL1	PD	CL2	89.95(2)	C1	N2	C3	108.3(1)
N1	C1	N2	108.4(2)	C1	N2	C5	125.7(1)
C1	N1	C2	108.8(1)	C3	N2	C5	126.0(1)
C1	N1	C4	125.8(2)	N2	C5	C6	112.1(1)
C2	N1	C4	125.4(2)	C5	C6	C7	112.9(2)
N1	C2	C3	107.3(2)	C6	C7	C8	114.8(2)