Orthometallated Palladium(II) Imine Complexes as Candidate Materials for the Biaxial Nematic Phase. Crystal and Molecular Structure of Three Palladium Imine Complexes

Viorel Cîrcu[a,b], Timothy J. K. Gibbs[a], Laurent Omnès[a], Peter N. Horton[c], Michael B. Hursthouse[c] and Duncan W. Bruce[a]*

[a] Department of Chemistry
University of York
Heslington
YORK
YO10 5DD
UK
Fax: (+44) 1904 432516
E-mail: db519@york.ac.uk

[b] Inorganic Chemistry Department
University of Bucharest
23 Dumbrava Rosie st.
020464, BUCHAREST
ROMANIA

[c] EPSRC Crystallographic Service
Department of Chemistry
University of Southampton
Highfield
SOUTHAMPTON
SO17 1BJ
UK

Electronic Supplementary Information

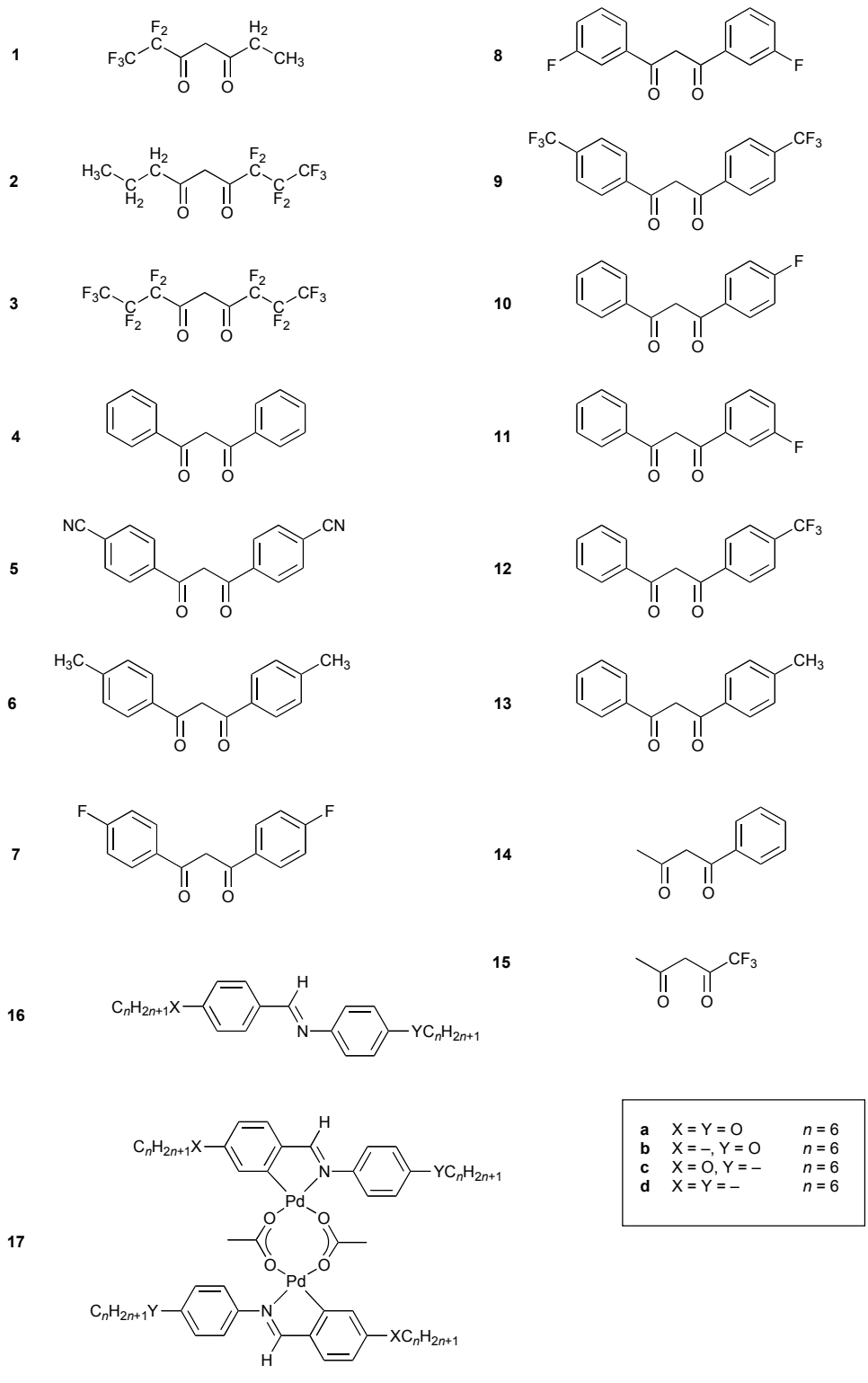

Figure S1 Ligands and complexes used in the study, presented structurally (see Figure 6 of main manuscript).

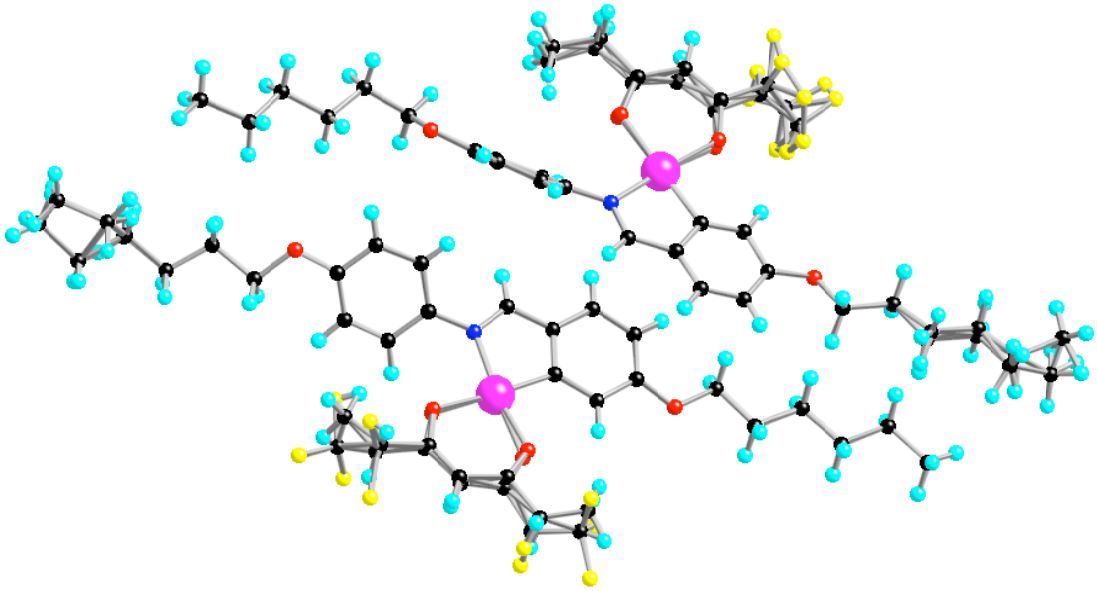

Figure S 2 View of Complex **1a** with disorder included

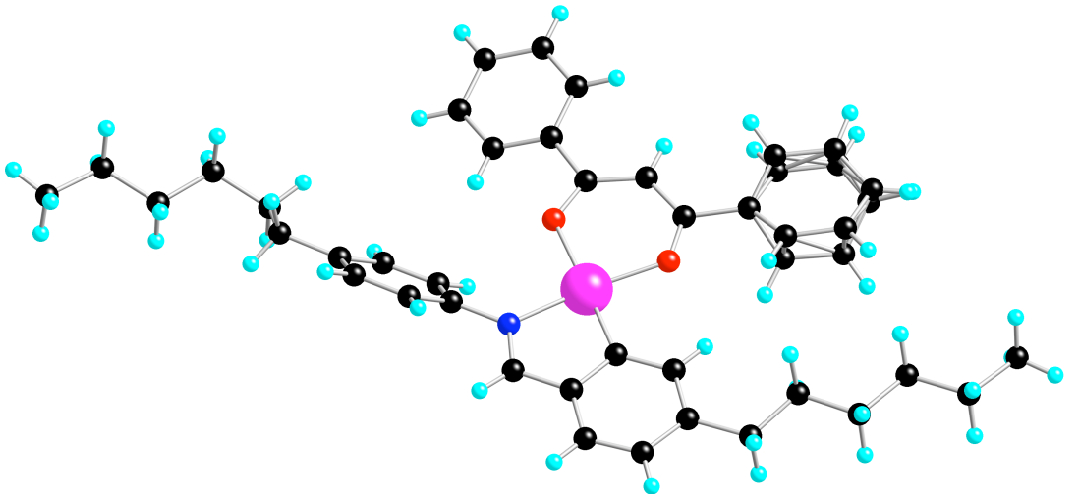

Figure S 3 View of one molecule in the unit cell of complex **4d** with disorder included

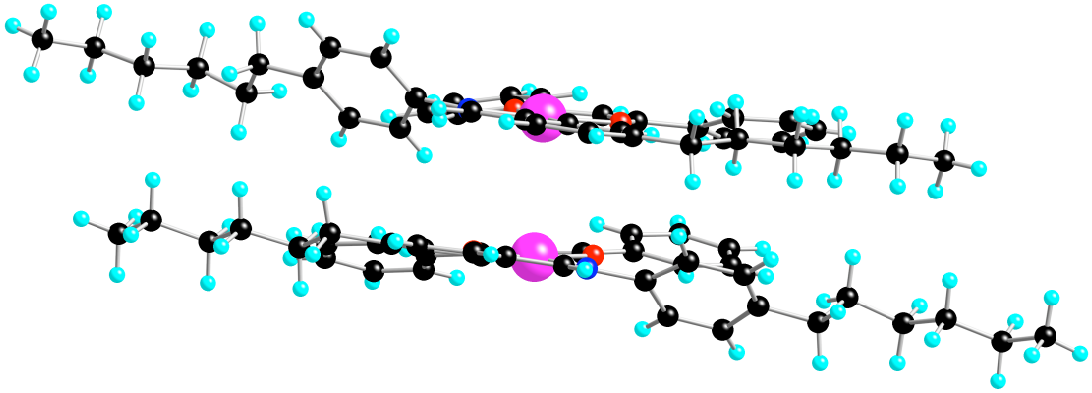

Figure S 4 Side-on view of compound **4d** (with disorder removed) showing Pd–Pd separation

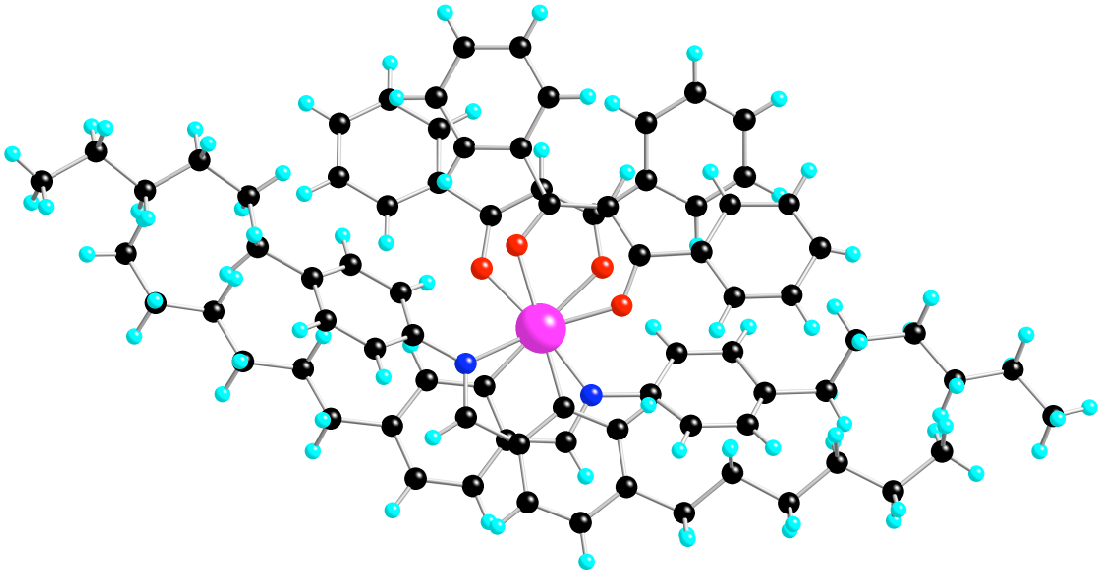

Figure S 5 Top view of compound **4d** (with disorder removed) with two palladium atoms overlaid

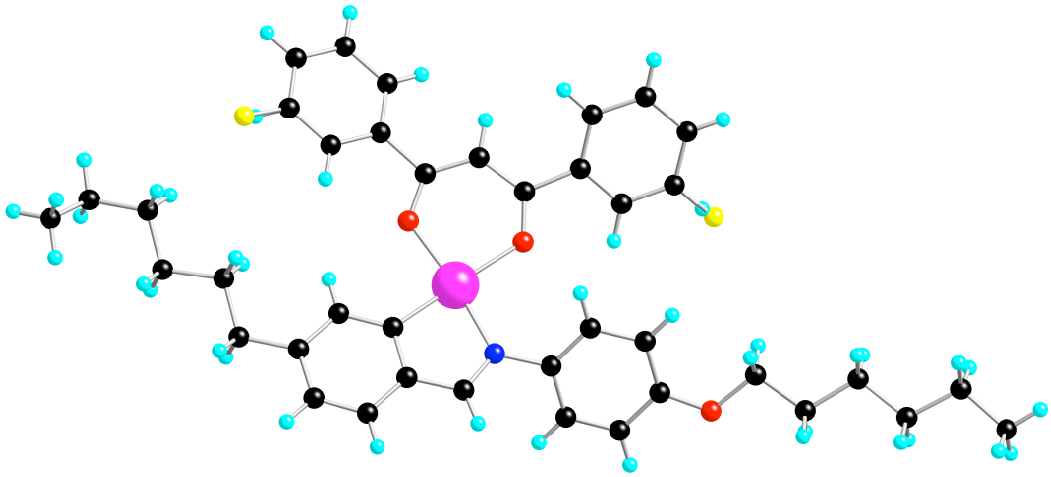

Figure S 6 View of complex **11b** with disorder included

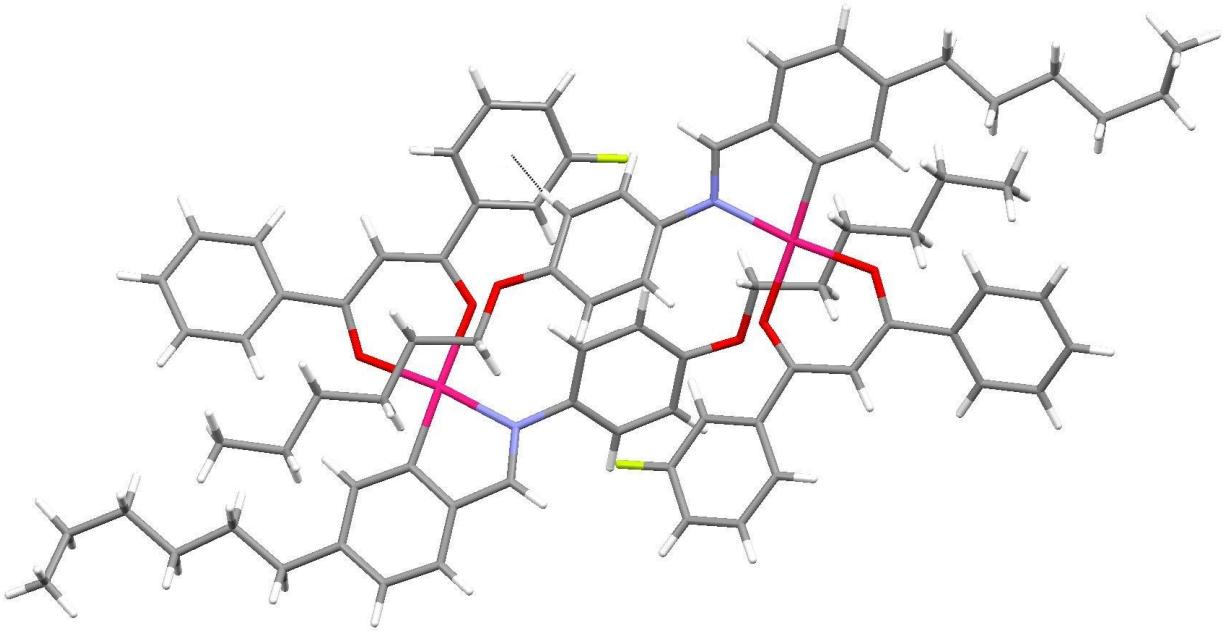

Figure S7 Complex 11b showing the intermolecular π–H bonding.

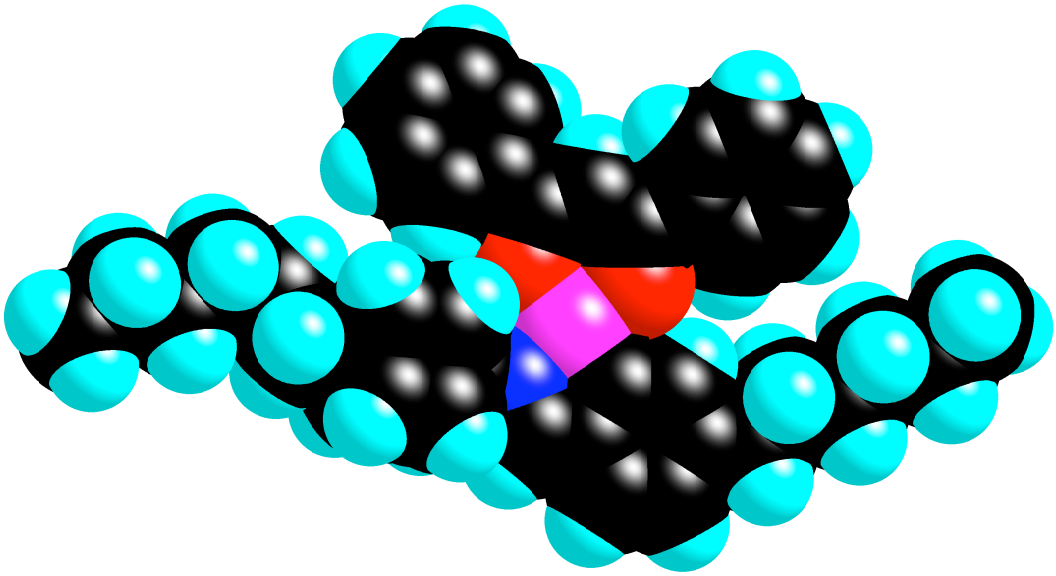

Figure S 8

Table. Analytical data for the new compounds

Compound	Yield/%	Calculated (Found)/%		
		C	H	N
1a	85	54.67(54.60)	5.73 (5.73)	1.99 (2.06)
1b	71	55.86 (55.70)	5.86 (5.85)	2.04 (1.69)
1c	59	55.86 (55.71)	5.86 (5.82)	2.04 (1.74)
1d	26	57.19 (56.89)	6.00 (5.73)	2.08 (1.93)
2a	80	45.91 (45.73)	3.53 (3.38)	2.23 (2.18)
2b	57	54.30 (54.03)	5.63 (5.70)	1.86 (1.53)
2c	74	54.30 (54.17)	5.63 (5.71)	1.86 (1.57)
2d	58	55.48 (55.36)	5.75 (5.59)	1.90 (1.83)
3a	44	45.68 (45.39)	3.95 (3.92)	1.57 (1.46)
4a	82	67.65 (67.22)	6.39 (6.34)	1.97 (1.62)
4b	64	69.20 (69.03)	6.53 (6.36)	2.02 (1.77)
4c	45	69.20 (69.33)	6.53 (6.75)	2.02 (1.46)
4d	51	70.84 (70.58)	6.69 (6.73)	2.07 (1.77)
5a	61	66.35 (66.31)	5.70 (5.75)	5.53 (5.13)
6	24	80.93 (81.42)	6.39 (6.86)	-
6a	45	68.24 (68.28)	6.82 (6.51)	1.89 (1.89)
6b	35	69.84 (69.66)	6.84 (6.98)	1.94 (1.85)

6c	59	69.84 (69.89)	6.84 (7.32)	1.94 (1.71)
6d	49	71.43 (71.24)	6.99 (7.10)	1.98 (1.90)
7	34	69.23 (69.03)	3.87 (3.83)	-
7a	68	59.47 (59.45)	3.83 (3.73)	2.31 (2.08)
7b	63	65.79 (65.62)	5.94 (5.79)	1.92 (1.67)
7c	56	65.79 (65.75)	5.94 (6.12)	1.92 (1.56)
7d	76	67.27 (67.22)	6.07 (6.23)	1.96 (1.69)
8	21	69.60 (69.60)	3.87 (3.88)	-
8a	32	64.30 (64.15)	5.94 (5.43)	1.87 (1.64)
8b	29	65.79 (65.70)	5.94 (6.04)	1.92 (1.78)
8c	56	65.79 (65.54)	5.94 (6.08)	1.92 (1.64)
8d	31	67.27 (67.35)	6.07 (6.33)	1.96 (1.83)
9	23	56.68 (56.81)	2.80 (2.80)	-
9a	29	59.40 (59.37)	5.46 (5.11)	1.65 (1.43)
9c	47	60.76 (60.54)	5.22 (5.32)	1.69 (1.58)
10	21	74.37 (74.42)	4.58 (4.10)	-
10a	61	65.88 (65.76)	6.22 (6.17)	1.92 (1.70)
10b	63	67.46 (67.10)	6.23 (6.00)	1.97 (1.75)
10c	55	67.46 (67.39)	6.23 (6.28)	1.97 (1.85)
10d	43	69.01 (68.84)	6.37 (6.41)	2.01 (1.92)
11	29	74.37 (74.42)	4.58 (4.62)	-
11a	68	65.97 (65.90)	6.09 (6.28)	1.92 (1.77)
11b	47	67.46 (67.12)	6.23 (6.02)	1.97 (1.75)
11c	48	67.46 (67.29)	6.23 (5.99)	1.97 (1.84)
11d	63	69.01 (68.89)	6.37 (6.27)	2.01 (1.91)
12	30	65.76 (65.71)	3.79 (3.75)	-
12a	60	63.28 (63.27)	5.70 (5.82)	1.80 (1.69)
12b	59	64.61 (64.16)	5.82 (5.90)	1.84 (1.68)
12c	56	64.61 (64.27)	5.82 (5.68)	1.84 (1.74)
12d	38	65.99 (65.81)	5.94 (5.81)	1.88 (1.77)
13	29	80.68 (80.68)	6.07 (5.92)	-
13a	63	67.99 (67.77)	6.54 (6.68)	1.93 (1.69)
13b	31	69.53 (69.49)	6.69 (6.48)	1.98 (1.92)
13c	44	69.53 (69.33)	6.69 (6.84)	1.98 (1.73)
13d	41	71.14 (70.94)	6.84 (7.04)	2.02 (1.98)
14a	77	64.56 (64.74)	7.12 (6.84)	2.15 (1.88)
14b	47	66.50 (66.53)	6.86 (7.03)	2.22 (2.15)
14c	53	66.50 (66.73)	6.86 (7.10)	2.22 (2.12)
14d	61	68.23 (68.49)	7.03 (7.35)	2.27 (2.20)
16b	42	82.14 (82.39)	9.65 (9.84)	3.83 (3.54)
17b	68	61.07 (61.22)	7.21 (7.27)	2.64 (2.53)
17c	73	61.07 (61.11)	7.21 (7.18)	2.64 (2.44)
17d	72	62.97 (62.79)	7.44 (7.84)	2.72 (2.52)