Electronic Supplementary Information for:

Chiral Single-Atom-Bridged Diphosphorus Ligands: Synthesis, Complexation and Catalysis

Javier Eusamio,[a,b] and Arnald Grabulosa[a,b,*]

[a]Departament de Química Inorgànica i Orgànica, Secció de Química Inorgànica, Universitat de Barcelona, Martí i Franquès, 1-11, E-08028, Barcelona, Spain. [b]Institut de Nanociència i Nanotecnologia (IN2UB), Universitat de Barcelona, E-08028, Barcelona, Spain.

Table of contents

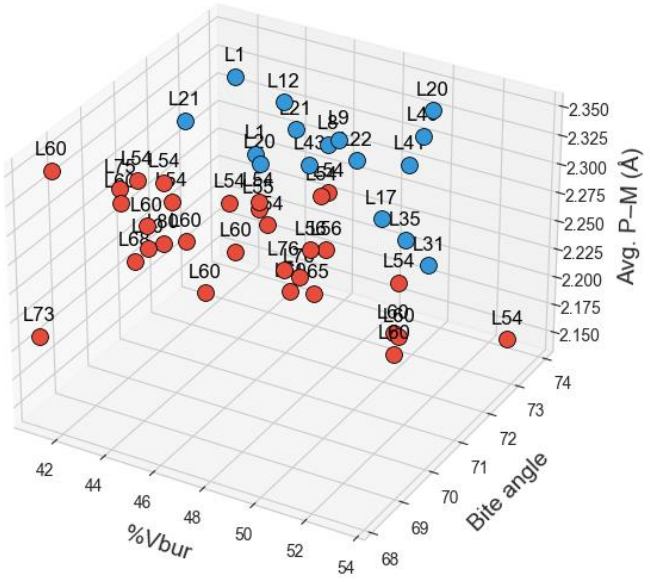

Figure S1

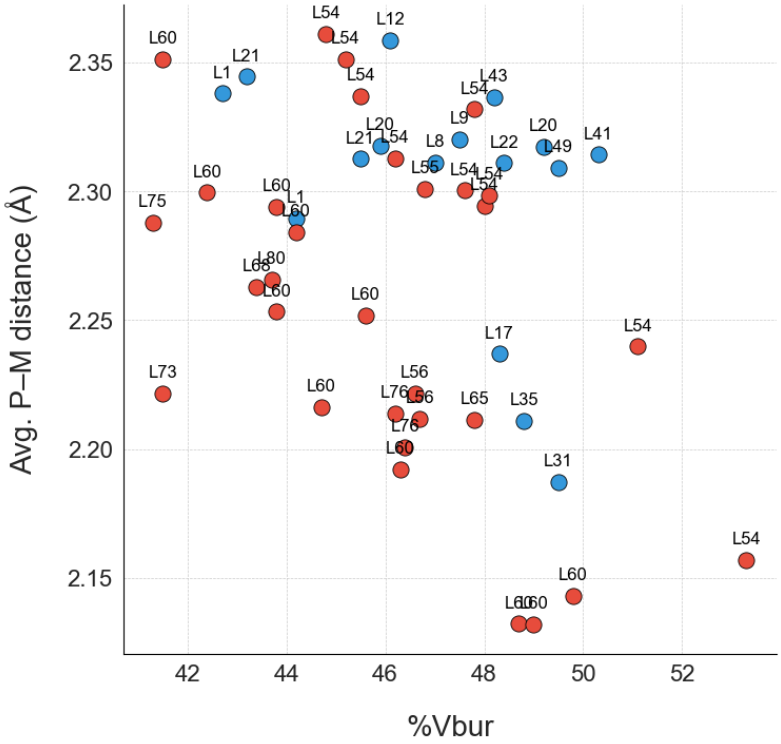

Figure S2

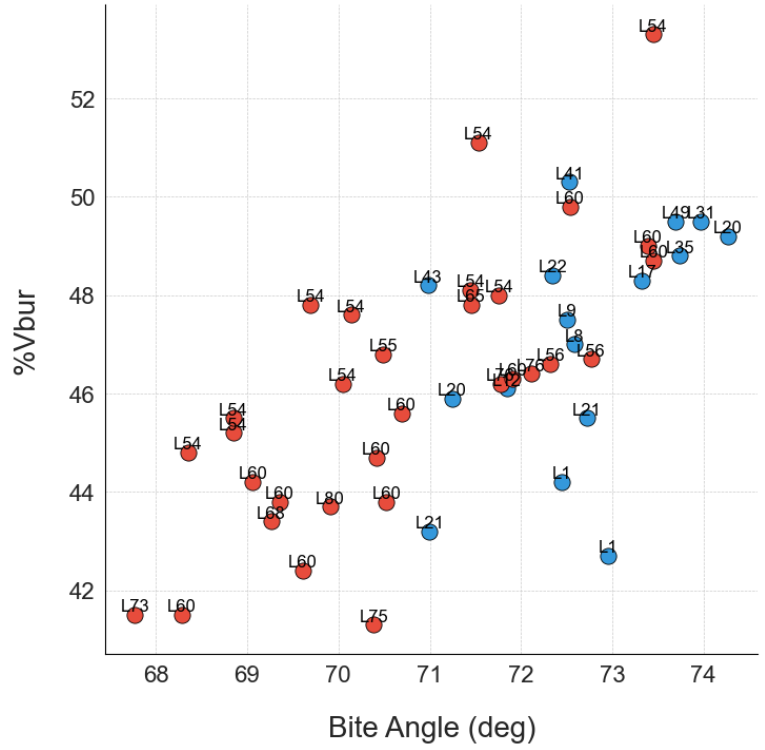

Figure S3

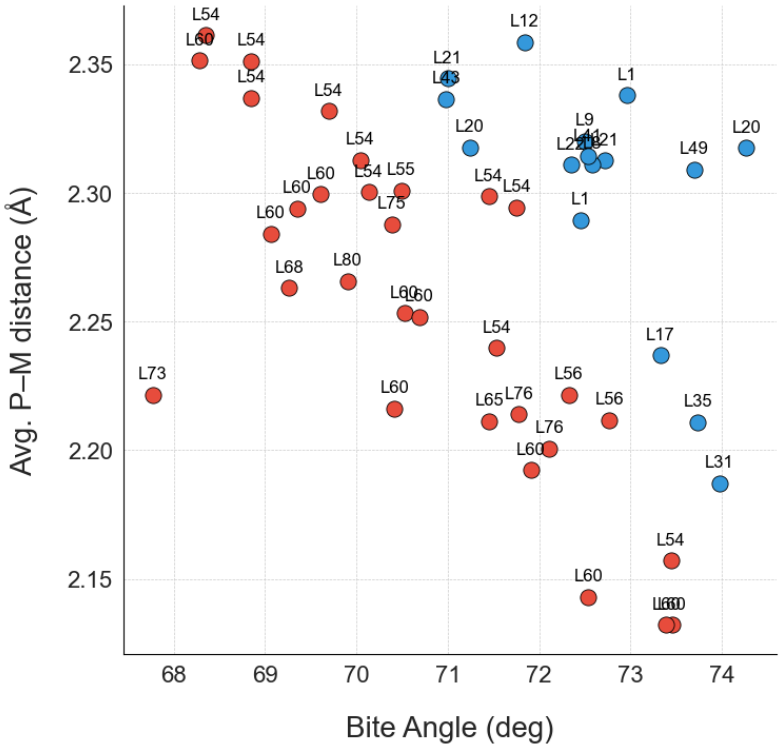

Figure S4

Table S1

Entry	CSD id.	Ligand	%Vbur	%Vbur SW	%Vbur NW	%Vbur SE	%Vbur NE	Bite angle	P1–M (Å)	P2–M (Å)	Avg. P–M (Å)	Metal center
1	QIXFIM	L1	42.7	48.7	38.3	37.9	45.9	72.96	2.35	2.32	2.34	Rh
2	QUKYEC	L1	44.2	48.2	40.5	39.6	48.6	72.45	2.29	2.29	2.29	Rh
3	TUGCUU	L12	46.1	41.9	48.3	50.9	43.3	71.84	2.34	2.38	2.36	Pd
4	SUPSII	L17	48.3	43.9	51.2	52.9	45.1	73.33	2.24	2.24	2.24	Pd
5	SUPSUU	L20	45.9	48.8	41.7	51.5	41.4	71.24	2.33	2.31	2.32	Pd
6	SUPTAB	L20	49.2	54.7	46.6	48.4	47.2	74.27	2.30	2.34	2.32	Pd
7	TEYKIV	L21	43.2	44.4	43.9	41	43.4	71.00	2.34	2.35	2.34	Ru
8	TEYKER	L21	45.5	45.3	47	49.7	39.8	72.72	2.33	2.30	2.31	Rh
9	TEYKAN	L22	48.4	44.2	49.6	51.9	48.1	72.35	2.34	2.29	2.31	Rh
10	XUMHAP	L31	49.5	49.1	52.8	51.6	44.5	73.97	2.20	2.18	2.19	Rh
11	MUDCOF	L35	48.8	44.6	42.8	53.3	54.3	73.74	2.26	2.16	2.21	Pt
12	MUDCIZ	L41	50.3	51	47.9	51.8	50.4	72.53	2.29	2.34	2.31	Rh
13	ZIQCAD	L43	48.2	48.5	50.4	49.2	44.7	70.98	2.36	2.31	2.34	Rh
14	PARMAY	L49	49.5	48.6	46.5	51.5	51.4	73.70	2.34	2.28	2.31	Rh
15	FEHWIB	L54	44.8	48	45.6	45.5	40.2	68.35	2.33	2.39	2.36	Ru
16	FEHWAT	L54	45.2	40.9	46.3	44.2	49.4	68.85	2.39	2.31	2.35	Rh
17	FEHWEX	L54	45.5	41	46.3	45.1	49.7	68.85	2.37	2.31	2.34	Ir
18	EHERIT	L54	46.2	52	45.6	45.4	41.9	70.04	2.29	2.34	2.31	Rh
19	POKFAY	L54	47.6	48.8	41	52.6	48.2	70.14	2.32	2.28	2.30	Rh
20	VUTGUO	L54	47.8	39.9	49.2	50.7	51.4	69.70	2.33	2.34	2.33	Rh
21	WOCVUH	L54	48	53.1	49.7	47.6	41.6	71.76	2.29	2.30	2.29	Pd
22	WOCWAO	L54	48.1	40.9	50.3	51.2	49.8	71.45	2.31	2.29	2.30	Pd
23	WOCVOB	L54	51.1	54.2	42.4	55.7	52	71.54	2.25	2.23	2.24	Pd
24	WOCVIV	L54	53.3	44.9	55.7	55.7	56.7	73.44	2.16	2.15	2.16	Ni
25	AHORUO	L55	46.8	47.2	41.3	52.3	46.5	70.49	2.33	2.28	2.30	Rh
26	QIQDID	L56	46.6	40	51.4	44.5	50.5	72.32	2.23	2.21	2.22	Pd

Entry	CSD id.	Ligand	%Vbur	%Vbur SW	%Vbur NW	%Vbur SE	%Vbur NE	Bite angle	P1–M (Å)	P2–M (Å)	Avg. P–M (Å)	Metal center
27	QIQDOJ	L56	46.7	40.3	51.1	44.8	50.5	72.77	2.22	2.21	2.21	Pt
28	EHUQED	L60	41.5	40.8	43.4	39.6	42.1	68.28	2.37	2.33	2.35	Ru
29	AXOSOV	L60	42.4	40.5	39.7	37.8	51.7	69.61	2.23	2.37	2.30	Ru
30	MOSQUG	L60	43.8	44.7	43.6	44.2	42.6	70.53	2.25	2.26	2.25	Ru
31	SEJZIR	L60	43.8	42.2	44.6	42.7	45.6	69.35	2.30	2.29	2.29	Ir
32	SEJZEN	L60	44.2	42.7	45.1	42.4	46.6	69.06	2.29	2.28	2.28	Rh
33	MOSQOA	L60	44.7	46.5	43.8	44.5	44	70.42	2.20	2.23	2.22	Ru
34	BIYVIO	L60	45.6	45.9	46.6	40.8	49.2	70.69	2.24	2.27	2.25	Pt
35	SEJZOX	L60	46.3	45.4	46.2	44.6	48.9	71.91	2.20	2.18	2.19	Fe
36	ZAWZUU	L60	48.7	53	44.2	51.1	46.5	73.45	2.13	2.14	2.13	Ni
37	HAFQAI	L60	49	46.2	51.4	44.3	54.2	73.39	2.14	2.13	2.13	Ni
38	PIDCAJ01	L60	49.8	44.9	52.4	55.6	46.3	72.54	2.14	2.15	2.14	Ni
39	YOKYEC	L65	47.8	53.5	43.5	49.8	44.6	71.45	2.21	2.21	2.21	Pd
40	AHAZOY	L68	43.4	40.7	45.1	42.8	45.2	69.27	2.25	2.28	2.26	Ru
41	YIBDOD	L73	41.5	42.2	41.9	39.2	42.8	67.77	2.20	2.24	2.22	Ru
42	YAKDOE	L75	41.3	41.1	50.1	37	37.1	70.39	2.28	2.30	2.29	Pd
43	BEPTAS	L76	46.2	43.5	49.4	43.5	48.4	71.78	2.21	2.22	2.21	Pd
44	BEPSUL	L76	46.4	44	49.5	43.6	48.6	72.11	2.20	2.20	2.20	Pt
45	BEWPEZ	L8	47	46.5	42.9	51.5	46.9	72.58	2.34	2.28	2.31	Rh
46	WAKYOA	L80	43.7	37.1	35.3	54	48.4	69.91	2.29	2.25	2.27	Rh
47	MOXFAJ	L9	47.5	48.3	41.9	52.5	47.3	72.50	2.35	2.29	2.32	Rh