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Table SI1 C-O, N-C, and C-C bond lengths in the structures of: (a) ^{Bz}LH·0.5H_2O and (b) ^{PhOMe}LH.

Figure SI1 Schematic representation of the intermolecular H-bonds in ^{Bz}LH·0.5H_2O.

Table SI2 C-O, N-C, and C-C bond lengths in: (a) **1**·4MeCN; (b) **2**·2MeOH; (c) **3**·2MeCN; and (d) **4**·2MeCN

Figure SI2. (a) Schematic representation of the intramolecular π-π interactions between the two ligands L and L^A of **2** in **2**·2MeOH. For clarity, only the rings involved in these interactions are shown. (b) A representation of the parameters involved in the interactions Ph/PhO and Ph/IM in **2**. The letter c is used for centroid of a ring and P for plane.

Table SI3 Geometrical parameters for the π-π stacking interactions in **2** in **2**·2MeOH.

Figure SI3. X-band EPR spectra of: (top) **1** and (bottom) **2** in CH_2Cl_2/DMF (9:1) at 77 K.

Table SI4. Spin-Hamiltonian parameters for the compounds **1** and **2** obtained by simulation of the X-band frozen solution spectra.

Table SI1a

Bond	Distance / Å		Distance / Å
O1-C19	1.349(7)	C13-C14	1.383(10)
O2-C9	1.356(10)	C14-C15	1.381(9)
O2-C24	1.369(16)	C15-C16	1.367(8)
O2-C24'	1.36(2)	C16-C17	1.386(9)
O3-C15	1.377(7)	C18-C23	1.407(8)
O3-C25	1.439(8)	C18-C19	1.393(8)
N2-C3	1.387(7)	C19-C20	1.410(8)
N2-C1	1.359(7)	C20-C21	1.403(8)
N5-C1	1.329(7)	C20-C26	1.537(9)
N5-C4	1.383(7)	C21-C22	1.413(8)
C1-C18	1.460(8)	C22-C23	1.376(8)
C3-C4	1.362(8)	C22-C30	1.533(8)
C3-C6	1.477(8)	C26-C28	1.533(12)
C4-C12	1.478(8)	C26-C27	1.537(12)
C6-C7	1.380(10)	C26-C29	1.539(11)
C6-C11	1.385(9)	C30-C32	1.517(9)
C7-C8	1.393(11)	C30-C33	1.537(10)
C8-C9	1.361(13)	C30-C32'	1.52(9)
C9-C10	1.357(11)	C30-C33'	1.53(5)
C10-C11	1.390(10)	C30-C31'	1.52(9)
C12-C13	1.396(8)	C30-C31	1.528(9)
C12-C17	1.386(9)		

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Table SI1b

	Distance /Å		Distance /Å
O1-C11	1.366(2)	C6A-C7A	1.381(3)
O1A-C11A	1.378(2)	C7A-C8A	1.398(3)
N2-C3	1.381(2)	C8A-C9A	1.378(3)
N2-C1	1.363(2)	C10A-C15A	1.403(2)
N5-C1	1.329(2)	C10A-C11A	1.398(2)
N5-C4	1.391(2)	C11A-C12A	1.414(3)
N2A-C1A	1.358(2)	C12A-C16A	1.543(3)
N2A-C3A	1.386(2)	C12A-C13A	1.387(3)
N5A-C1A	1.329(2)	C13A-C14A	1.407(3)
N5A-C4A	1.392(2)	C14A-C15A	1.376(3)
C1-C10	1.460(3)	C14A-C20A	1.532(3)
C3-C4	1.400(3)	C16A-C17A	1.533(3)
C3-C6	1.391(3)	C16A-C19A	1.535(3)
C4-C9	1.400(3)	C16A-C18A	1.539(3)
C6-C7	1.378(3)	C20A-C23A	1.544(3)
C7-C8	1.404(3)	C20A-C21A	1.528(3)
C8-C9	1.383(3)	C13-C14	1.401(3)
C10-C11	1.404(3)	C14-C20	1.535(3)
C10-C15	1.402(2)	C14-C15	1.383(3)
C11-C12	1.409(3)	C16-C19	1.530(3)
C12-C16	1.541(3)	C16-C18	1.537(3)
C12-C13	1.391(3)	C16-C17	1.538(3)
C1A-C10A	1.459(2)	C20-C23	1.530(3)
C3A-C6A	1.387(3)	C20-C21	1.526(3)
C3A-C4A	1.407(3)	C20-C22	1.531(3)
C4A-C9A	1.390(3)		

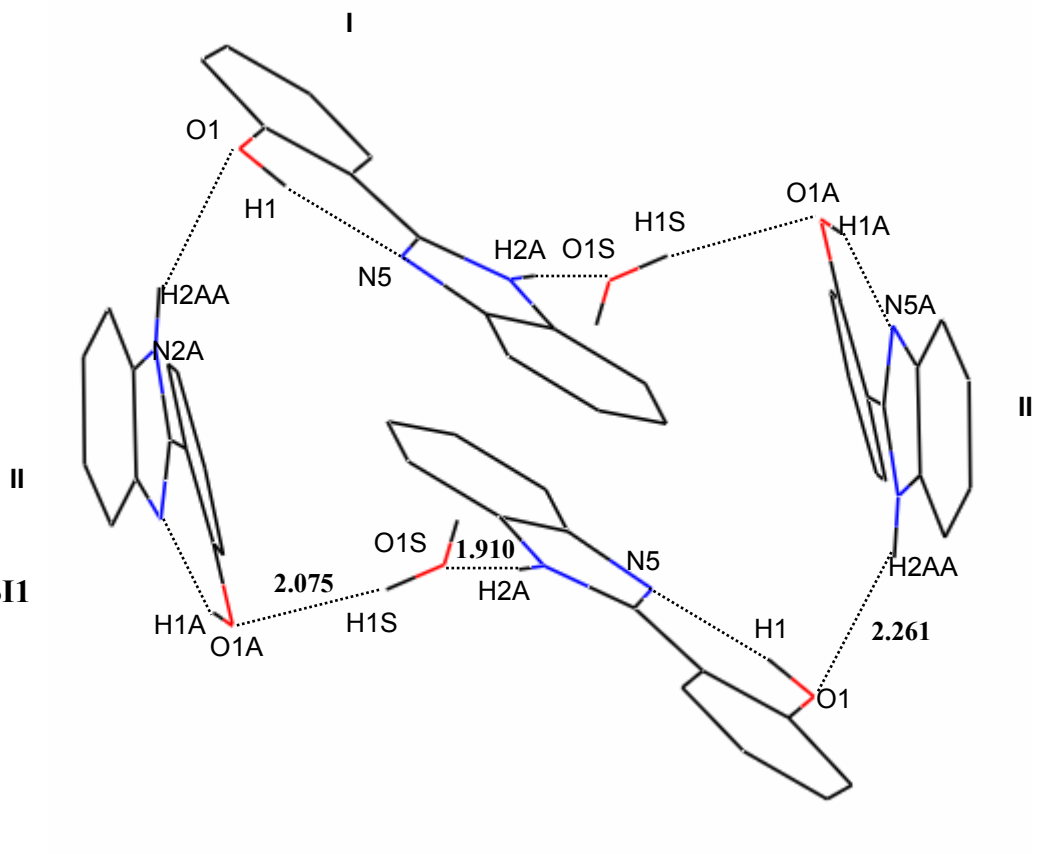

Figure SI1

Table SI2a

Bond	Distance / Å	Bond	Distance / Å	Bond	Distance / Å
C(1)-N(5)	1.346(4)	C(16)-C(19)	1.530(5)	C(11A)-C(12A)	1.427(5)
C(1)-N(2)	1.364(4)	C(16)-C(18)	1.532(5)	C(12A)-C(13A)	1.383(5)
C(1)-C(10)	1.449(5)	C(16)-C(17)	1.547(6)	C(12A)-C(16A)	1.534(5)
O(1)-C(11)	1.325(4)	C(20)-C(21)	1.514(6)	C(13A)-C(14A)	1.408(5)
N(2)-C(3)	1.382(5)	C(20)-C(23)	1.536(6)	C(14A)-C(15A)	1.377(5)
C(3)-C(4)	1.390(5)	C(20)-C(22)	1.543(6)	C(14A)-C(20A)	1.549(5)
C(3)-C(9)	1.396(5)	O(1A)-C(11A)	1.329(4)	C(16A)-C(19A)	1.533(5)
C(4)-C(6)	1.381(5)	C(1A)-N(5A)	1.341(4)	C(16A)-C(18A)	1.540(5)
C(4)-N(5)	1.406(4)	C(1A)-N(2A)	1.358(4)	C(16A)-C(17A)	1.540(5)
C(6)-C(7)	1.378(5)	C(1A)-C(10A)	1.456(5)	C(20A)-C(23A)	1.516(6)
C(7)-C(8)	1.399(6)	N(2A)-C(3A)	1.382(4)	C(20A)-C(21A)	1.521(6)
C(8)-C(9)	1.379(5)	C(3A)-C(9A)	1.391(5)	C(20A)-C(22A)	1.543(6)
C(10)-C(15)	1.407(5)	C(3A)-C(4A)	1.396(5)	N(1S)-C(1S)	1.133(4)
C(10)-C(11)	1.414(5)	C(4A)-C(6A)	1.390(5)	C(1S)-C(2S)	1.458(5)
C(11)-C(12)	1.429(5)	C(4A)-N(5A)	1.405(4)	N(2S)-C(3S)	1.120(6)
C(12)-C(13)	1.379(5)	C(6A)-C(7A)	1.391(5)	C(3S)-C(4S)	1.440(6)
C(12)-C(16)	1.534(5)	C(7A)-C(8A)	1.400(5)	N(3S)-C(5S)	1.136(5)
C(13)-C(14)	1.412(5)	C(8A)-C(9A)	1.378(5)	C(5S)-C(6S)	1.456(5)
C(14)-C(15)	1.374(5)	C(10A)-C(15A)	1.403(5)	N(4S)-C(7S)	1.146(6)
C(14)-C(20)	1.541(5)	C(10A)-C(11A)	1.417(5)	C(7S)-C(8S)	1.454(7)

TableSI2b

Bond	Distance / Å	Bond	Distance / Å
Cu(1)-O(1)	1.890(4)	O(3A)-C(15A)	1.377(8)
Cu(1)-O(1A)	1.917(4)	O(3A)-C(25A)	1.420(8)
Cu(1)-N(5)	1.946(5)	O(1SA)-C(1SA)	1.416(8)
Cu(1)-N(5A)	1.973(5)	O(1S)-C(1S)	1.439(9)
O(1)-C(19)	1.323(8)	N(2)-C(1)	1.369(9)
O(1A)-C(19A)	1.344(8)	N(2)-C(3)	1.381(8)
O(2)-C(9)	1.366(8)	N(2A)-C(3A)	1.383(9)
O(2)-C(24)	1.428(8)	N(2A)-C(1A)	1.332(9)
O(2A)-C(9A)	1.368(7)	N(5)-C(1)	1.336(9)
O(2A)-C(24A)	1.416(8)	N(5)-C(4)	1.385(8)
O(3)-C(15)	1.372(8)	N(5A)-C(4A)	1.407(8)
O(3)-C(25)	1.420(8)	N(5A)-C(1A)	1.354(9)

Table SI2c

Bond	Distance / Å	Bond	Distance / Å
O(1)-C(11)	1.331(2)	C(11)-C(12)	1.431(3)
C(1)-N(5)	1.343(2)	C(12)-C(13)	1.387(3)
C(1)-N(2)	1.362(2)	C(12)-C(16)	1.544(3)
C(1)-C(10)	1.459(3)	C(13)-C(14)	1.396(3)
N(2)-C(3)	1.384(2)	C(14)-C(15)	1.382(3)
C(3)-C(6)	1.390(3)	C(14)-C(20)	1.541(3)
C(3)-C(4)	1.398(3)	C(16)-C(19)	1.539(3)
C(4)-N(5)	1.389(2)	C(16)-C(18)	1.539(3)
C(4)-C(9)	1.394(3)	C(16)-C(17)	1.542(3)
C(6)-C(7)	1.379(3)	C(20)-C(23)	1.534(3)
C(7)-C(8)	1.401(3)	C(20)-C(22)	1.534(3)
C(8)-C(9)	1.384(3)	C(20)-C(21)	1.538(3)
C(10)-C(15)	1.405(2)	N(1S)-C(1S)	1.131(3)
C(10)-C(11)	1.425(3)	C(1S)-C(2S)	1.457(3)

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Table SI2d

Bond	Distance / Å	Bond	Distance / Å	Bond	Distance / Å
O(1)-C(19)	1.322(2)	C(18)-C(19)	1.423(3)	C(7A)-C(8A)	1.369(3)
C(1)-N(5)	1.342(2)	C(19)-C(20)	1.431(3)	C(8A)-C(9A)	1.389(3)
C(1)-N(2)	1.365(2)	C(20)-C(21)	1.386(3)	C(9A)-C(10A)	1.386(3)
C(1)-C(18)	1.469(3)	C(20)-C(26)	1.542(3)	C(10A)-C(11A)	1.389(3)
N(2)-C(3)	1.384(2)	C(21)-C(22)	1.404(3)	C(12A)-C(13A)	1.384(3)
O(2)-C(9)	1.371(2)	C(22)-C(23)	1.382(3)	C(12A)-C(17A)	1.397(3)
O(2)-C(24)	1.428(3)	C(22)-C(30)	1.540(3)	C(13A)-C(14A)	1.392(3)
C(3)-C(4)	1.369(3)	C(26)-C(27)	1.538(3)	C(14A)-C(15A)	1.382(3)
C(3)-C(6)	1.473(3)	C(26)-C(29)	1.542(3)	C(15A)-C(16A)	1.389(3)
O(3)-C(15)	1.397(3)	C(26)-C(28)	1.545(3)	C(16A)-C(17A)	1.383(3)
O(3)-C(25)	1.404(5)	C(30)-C(32)	1.516(4)	C(18A)-C(23A)	1.405(3)
O(3')-C(15)	1.395(5)	C(30)-C(31)	1.532(4)	C(18A)-C(19A)	1.429(3)
O(3')-C(25')	1.412(8)	C(30)-C(33)	1.532(4)	C(19A)-C(20A)	1.432(3)
C(4)-N(5)	1.390(2)	O(1A)-C(19A)	1.318(2)	C(20A)-C(21A)	1.395(3)
C(4)-C(12)	1.479(3)	C(1A)-N(5A)	1.344(2)	C(20A)-C(26A)	1.540(3)
C(6)-C(11)	1.394(3)	C(1A)-N(2A)	1.354(3)	C(21A)-C(22A)	1.398(3)
C(6)-C(7)	1.398(3)	C(1A)-C(18A)	1.469(3)	C(22A)-C(23A)	1.379(3)
C(7)-C(8)	1.377(3)	N(2A)-C(3A)	1.382(2)	C(22A)-C(30A)	1.547(3)
C(8)-C(9)	1.397(3)	O(2A)-C(9A)	1.367(3)	C(26A)-C(29A)	1.538(4)
C(9)-C(10)	1.389(3)	O(2A)-C(24A)	1.424(3)	C(26A)-C(27A)	1.539(3)
C(10)-C(11)	1.395(3)	C(3A)-C(4A)	1.370(3)	C(26A)-C(28A)	1.545(4)
C(12)-C(17)	1.382(3)	C(3A)-C(6A)	1.469(3)	C(30A)-C(31A)	1.526(3)
C(12)-C(13)	1.394(3)	O(3A)-C(15A)	1.372(3)	C(30A)-C(33A)	1.534(3)
C(13)-C(14)	1.387(3)	O(3A)-C(25A)	1.427(3)	C(30A)-C(32A)	1.538(3)
C(14)-C(15)	1.378(4)	C(4A)-N(5A)	1.389(3)	C(1S)-C(2S)	1.467(4)
C(15)-C(16)	1.377(4)	C(4A)-C(12A)	1.474(3)	C(2S)-N(3S)	1.138(3)
C(16)-C(17)	1.398(3)	C(6A)-C(11A)	1.386(3)	C(4S)-C(5S)	1.468(3)
C(18)-C(23)	1.409(3)	C(6A)-C(7A)	1.402(3)	C(5S)-N(6S)	1.122(3)

Figure SI2a

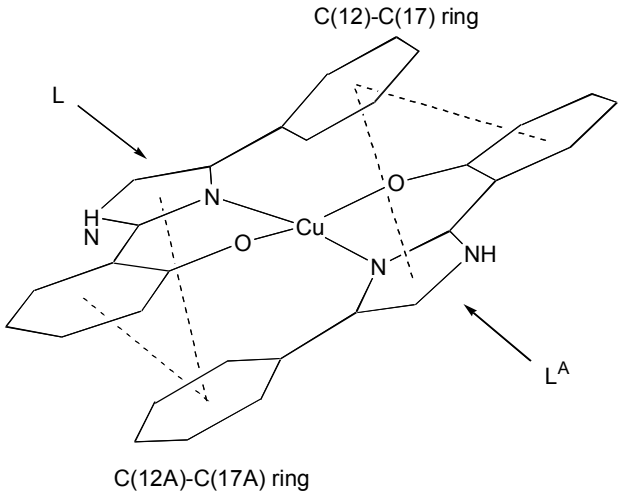

Figure SI2b

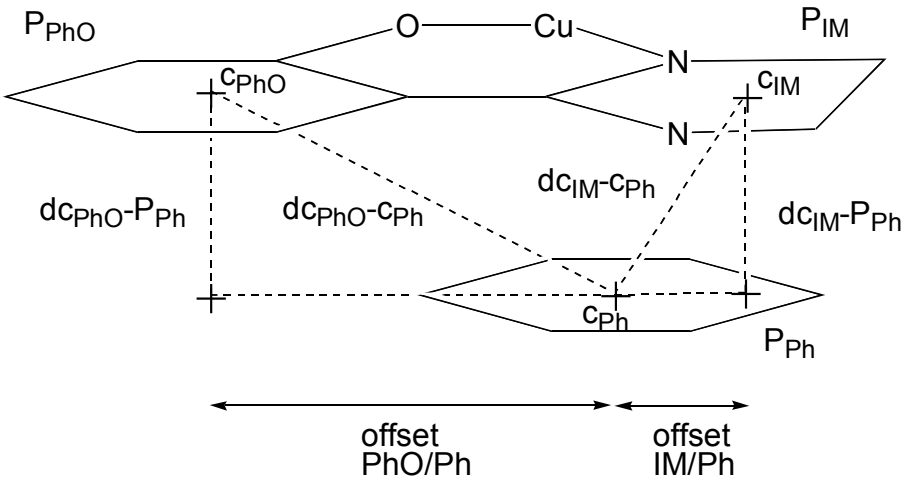

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Table SI3

Interaction	Angle between P_{Ph} and P_{IM} /°	$dc_{IM}c_{Ph}$ /Å	$dc_{IM}P_{Ph}$ /Å	Offset Ph/IM /Å	Angle between P_{Ph} and P_{IM} /°	$dc_{PhO}c_{Ph}$ /Å	$dc_{PhO}P_{Ph}$ /Å	Offset Ph/IM/ Å	Angle between PhO and IM /°	
									L	L(A)
Ph/IM(A)	15.2	3.54	3.46	0.75						
Ph(A)/IM	14.0	3.43	3.42	0.19						
Ph/PhO(A)					10.3	4.62	3.59	2.91		
Ph(A)/PhO					9.4	5.40	3.25	4.30		
									8.1	21.7

Figure SI3.

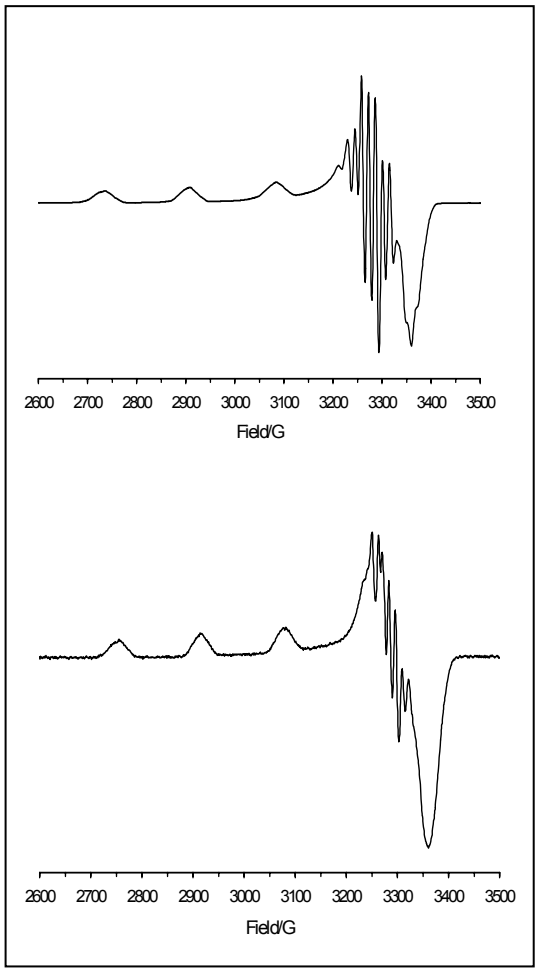

Table SI4.

Compounds	g_{zz}	$g_{xx/yy}$	$A_{zz}\{^{63,65}Cu\}$/G	$A_{xx/yy}\{^{63,65}Cu\}$/G	$a_{zz}\{^{14}N\}$/G	$a_{xx/yy}\{^{14}N\}$/G
1	2.254	2.048	165	21	10	13
2	2.254	2.048	164	19	10	13