Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supplementary Information

"THE BINUCLEAR DUAL EMITTER $[Br(CO)_3Re(P\ldots N)(N\ldots P)Re(CO)_3Br]$ (P…N): 3-CHLORO-6-(4-DIPHENYLPHOSPHINYL)BUTHOXYPYRIDA-ZINE), A NEW BRIDGING *P,N*-BIDENTATE LIGAND RESULTING FROM THE RING OPENING OF TETRAHYDROFURAN"

by the authors:

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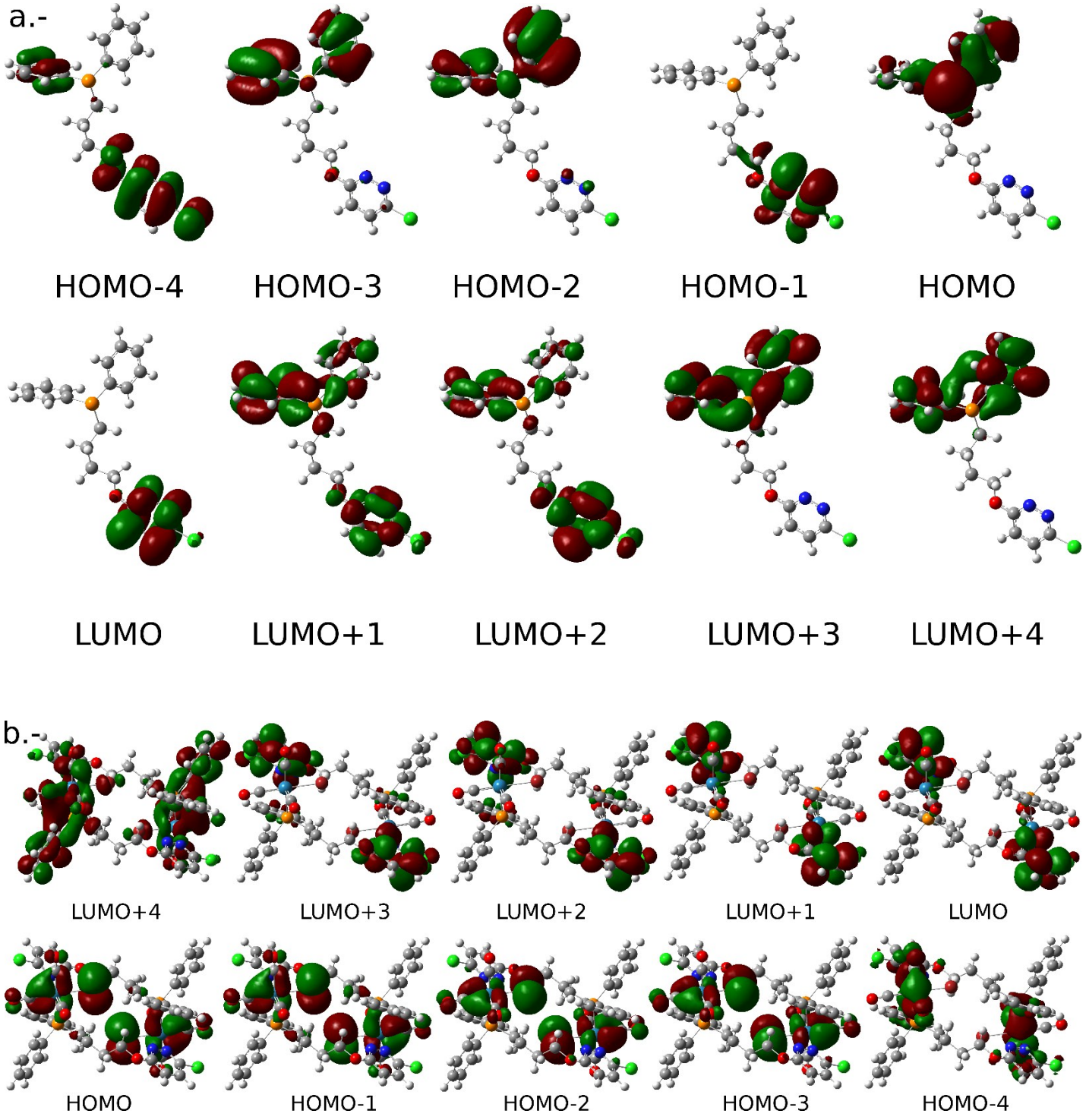

Figure S1. DFT computed frontier and near frontier orbitals for (**a.-**) **P…N** and (**b.-**) **BrRe(P…N)(N…P)ReBr**.

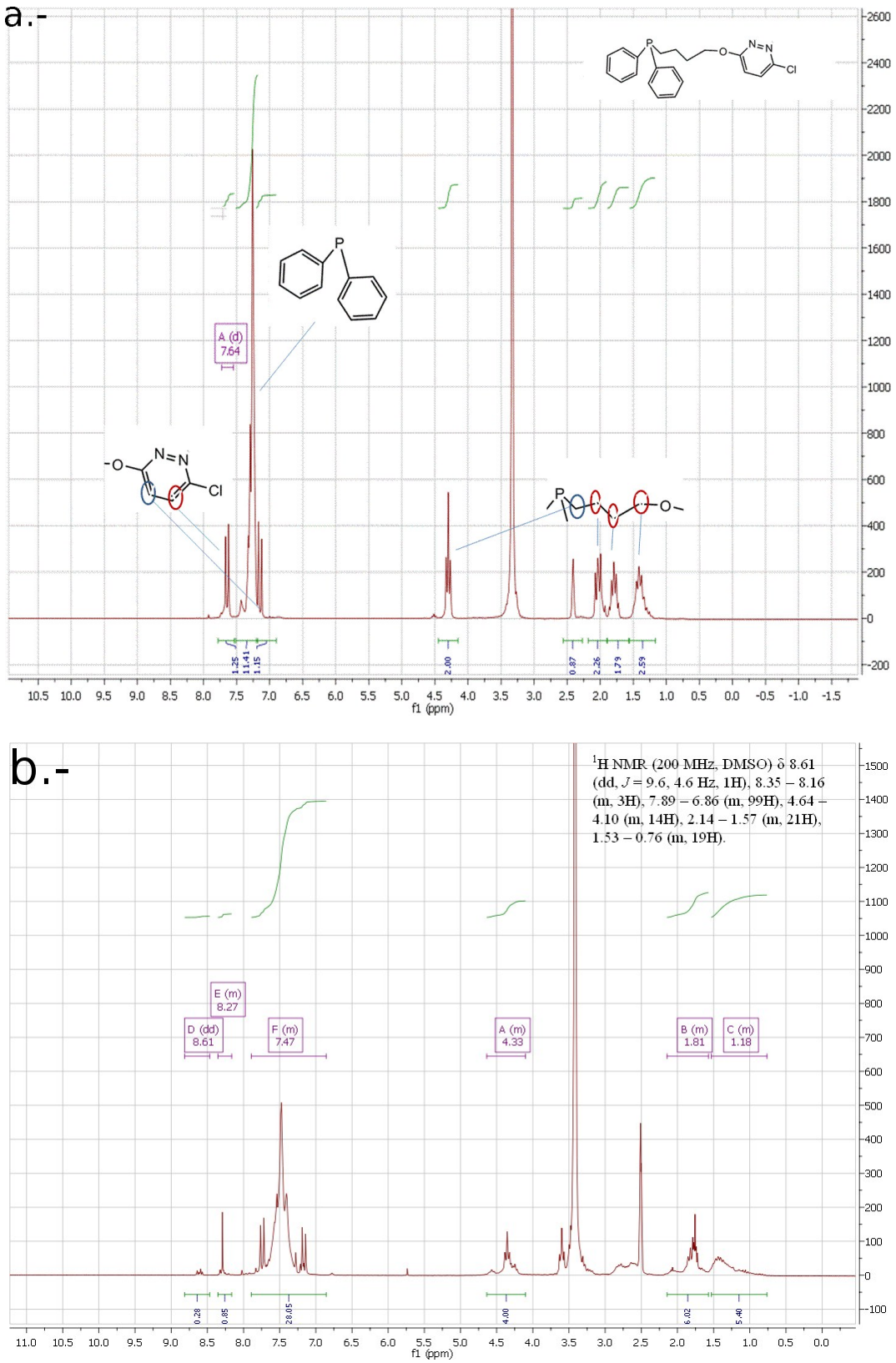

Figure S2. ^{1}HNMR spectra determined for (**a.-**) **P…N** and (**b.-**) **BrRe(P…N)(N…P)ReBr**.

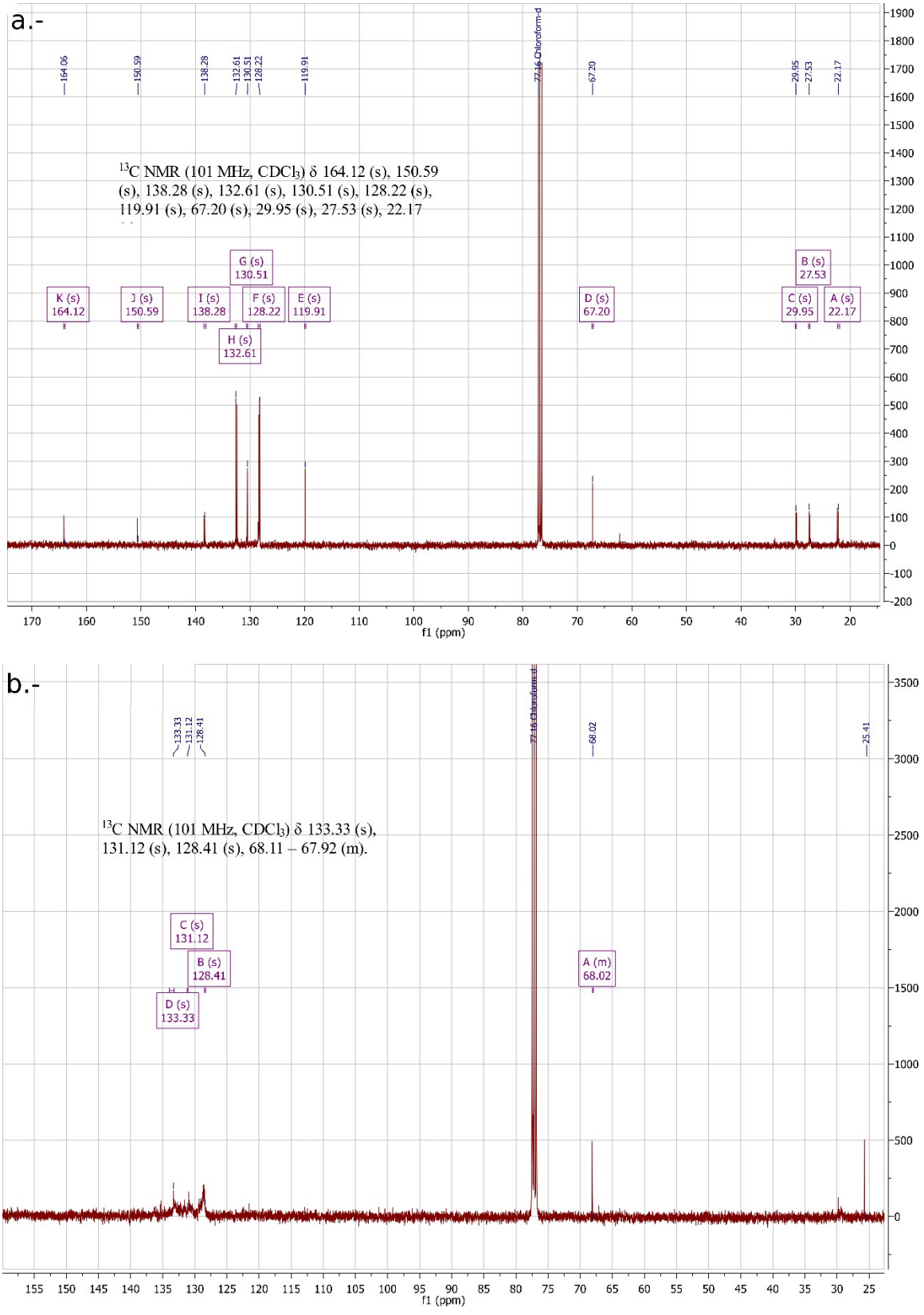

Figure S3. ^{13}CNMR spectra determined for (**a.-**) **P…N** and (**b.-**) **BrRe(P…N)(N…P)ReBr**.

Table S1. Crystal data and structure refinement [**BrRe(P…N)(N…P)ReBr**] · ($CHCl_3$).

FW/uma	3121.49
Crystal System	Monoclinic
Space Group	$P2_1/n$
a (Å)	14.610(2)
b (Å)	16.549(3)
c (Å)	14.945(2)
β (°)	106.963(2)
V (Å^3)	3456.2(9)
Z	1
d (g cm^{-3})	1.501
μ (mm^{-1})	4.94
F000	1499
θ range	1.72 to 26.00
hkl range	-18 ≤ h ≤ 18
	-20 ≤ k ≤ 20
	-18 ≤ l ≤ 18
N_{tot}, N_{uniq}	25442, 6779(0.157),
(R_{int}), N_{obs}	3733
Refinement Parameters	379
GOF	1.00
R1, wR2 (obs)	0.064, 0.169
Max. and min Δρ	0.86,-1.17

Table S2. Bond distances (Å) for **BrRe(P…N)(N…P)ReBr**, [**BrRe(P…N)(N…P)ReBr**]$^{+}$ and [**BrRe(P…N)(N…P)ReBr**]$^{-}$ as determined from crystallographic data and/or computed from DFT.

	BrRe(P…N)(N…P)ReBr			[**BrRe(P…N)(N…P)ReBr**]$^{+}$	[**BrRe(P…N)(N…P)ReBr**]$^{-}$
Distance	**X-rays**	**DFT**		**DFT**	**DFT**
		Gas Phase	**PCM = DCM**	**Gas Phase**	**Gas Phase**
Re1—Br1	2.6442(13)	2.708	2.720	2.623	2.724
Re1—N1	2.213(10)	2.325	2.319	2.320	2.288
Re1—P1	2.491(3)	2.568	2.579	2.583	2.574
Re1—C17	1.865(11)	1.918	1.916	1.925	1.918
Re1—C18	1.996(19)	1.950	1.945	1.973	1.944
Re1—C19	1.858(13)	1.912	1.908	1.938	1.907
Re1···Re1	9.1467(14)	9.466	9.684	9.509	9.564