

## Synthesis and first complexes of C<sup>4/5</sup> P-bifunctional imidazole-2-thiones

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### Supporting information

Table S1. Crystallographic Data for Compounds **5c** and **7d**

Compound	<b>5c</b>	<b>7d</b>
Crystal system	Monoclinic	Triclinic
Space group	P 21/n	P -1
a (Å)	9.3636(8)	11.6761(9)
b (Å)	34.410(3)	11.7150(11)
c (Å)	9.3807(8)	12.7206(13)
$\beta$ (°)	117.124(2)	104.629(3)
V (Å <sup>3</sup> )	2690.1(4)	1442.7(2)
Z	4	2
$d_c$ (g cm <sup>-3</sup> )	1.335	1.313
$\mu$ (mm <sup>-1</sup> )	0.267	0.256
F(000)	1136	600
Crystal size(mm)	0.30 x 0.30 x 0.24	0.08 x 0.04 x 0.03
Reflections collected	27883	12940
Reflections unique	6484	5525
Mo K $\alpha$ radiation ( $\lambda$ , Å)	0.71073	0.71073
Final R indices(R1)	0.0377	0.0436
wR2	0.0933	0.0961
R indices (all data) R1	0.0470	0.0762
wR2	0.0978	0.1079
GOF	1.067	1.037
Parameters	337	354

Table S2. Crystallographic Data for Compounds **8b**, **9a** and **13**

Compound	<b>8b</b>	<b>9a</b>	<b>13</b>
Crystal system	orthorhombic	Monoclinic	Monoclinic
Space group	Pna2 <sub>1</sub>	C 2/c	P 21/c
a (Å)	12.4616(3)	15.6164(16)	11.1582(2)
b (Å)	20.6622(6)	12.2568(12)	26.3418(5)
c (Å)	12.8212	14.9796(14)	17.2063
β (°)	-	112.742(3)	116.5660
V (Å <sup>3</sup> )	3301.26(16)	2644.3(5)	4523.44(15)
Z	4	4	4
d <sub>c</sub> (g·cm <sup>-3</sup> )	1.345	1.408	1.505
μ (mm <sup>-1</sup> )	0.294	0.424	0.876
F(000)	1392	1168	2096
Crystal size(mm)	0.32 x 0.32 x 0.16	0.60 x 0.30 x 0.10	0.09 x 0.07 x 0.02
Reflections collected	17943	17773	58084
Reflections unique	7777	3185	10910
Mo Kα radiation (λ, Å)	0.71073	0.71073	0.71073
Final R indices(R1)	0.0377	0.0286	0.0400
wR2	0.1012	0.0741	0.0973
R indices (all data) R1	0.0459	0.0327	0.0617
wR2	0.1046	0.0767	0.1052
GOF	1.038	1.047	1.048
Parameters	416	165	499