Supporting Information File for manuscript:

Structural diversity and tetrel bonding significance in lead(II) complexes with pyrazoylisonicotinoylhydrazone and varied anionic co-ligands

Ghodrat Mahmoudi[a], Isabel García-Santos[b]*, Roi Fernández-Vázquez[b], Rosa M. Gomila[c], Alfonso Castiñeiras[b], Esmail Doustkhah,[d] Ennio Zangrando[e], and Antonio Frontera*[c]

a. Department of Chemistry, Faculty of Science, University of Maragheh, P.O. Box 55136-83111, Maragheh, Iran.
b. Departamento de Química Inorgánica, Facultad de Farmacia, Universidad de Santiago de Compostela, E-15782 Santiago de Compostela, Spain. E-mail: isabel.garcia@usc.es.
c. Department of Chemistry, Universitat de les Illes Balears. Crta de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), SPAIN.
d. Chemistry Department, Faculty of Engineering and Natural Sciences, Istinye University, Sarıyer, Istanbul 34396, Turkey
e. Department of Chemical and Pharmaceutical Sciences, University of Trieste, Via L. Giorgieri 1, 34127 Trieste, Italy

Table of contents:

Table S1. Crystallographic Data and Details of Refinements for complexes **1 - 4**.

	1	**2**	**3**	**4**
empirical formula	$C_{11}H_9N_9OPb$	$C_{12}H_9N_7OPbS$	$C_{11}H_9N_7O_3Pb$	$C_{11}H_9N_7O_4Pb$
fw	490.46	506.51	494.44	510.44
cryst system	monoclinic	monoclinic	monoclinic	monoclinic
space group	$P\,2_1/c$	$P\,2_1/c$	$P\,2_1/c$	$P\,2_1/c$
a (Å)	8.7307(3)	8.4135(7)	7.1869(3)	7.1282(3)
b (Å)	16.6328(7)	16.6666(12)	18.1539(7)	16.9244(6)
c (Å)	9.6082(4)	10.1721(7)	10.3088(4)	12.1283(5)
β (°)	100.1460(10)	95.905(2)	97.142(2)	104.3430(10)
V (Å^3)	1373.45(9)	1418.81(18)	1334.56(9)	1417.56(10)
Z	4	4	4	4
D_{calcd} (mg/m^3)	2.372	2.371	2.461	2.392
μ(Mo-Kα) (mm^{-1})	12.302	12.051	12.668	11.936
F(000)	912	944	920	952
θ range (°)	2.48 - 30.51	2.35 - 27.48	2.24 - 28.28	2.41 to 26.37
Collected refls	41121	24267	28327	27636
Indep reflections	4198	3231	3308	2895
R_{int}	0.0298	0.0577	0.0476	0.0705
Obsrvd refls $I > 2\sigma(I)$	3849	2807	3013	2500
Parameters	205	205	199	214
GOF on F^2	1.090	1.032	1.073	1.228
$R1$ ($I > 2\sigma(I)$) [a]	0.0144	0.0214	0.0199	0.0341
$wR2$ ($I > 2\sigma(I)$) [a]	0.0303	0.0422	0.0456	0.0849
residuals (e Å^{-3})	0.703, -0.807	0.762, -0.798	0.735, -1.333	2.266, -1.212

[a] $R1 = \Sigma \, | \, |Fo| - |Fc| \, | \, / \Sigma |Fo|$, $wR2 = \Sigma \, w \, (Fo^2 - Fc^2)^2 / \Sigma w \, (Fo^2)^2 \,]^{½}$

Table S2. Hydrogen bond parameters (Å /°) for complexes **1** - **4**.

D-H	d(D-H)	d(H..A)	d(D..A)	<DHA	A	Symmetry code
Complex **1**						
N5-H5a	0.77(3)	2.26(3)	2.604(2)	108(2)	N3	intra
N5-H5b	0.82(3)	2.10(3)	2.907(3)	170(2)	N6	1+x,1/2-y,1/2+z
C2-H2	0.94	2.59	3.426(3)	148	N9	3-x,-y,2-z
C3-H3	0.94	2.46	3.168(2)	132	O1	1+x,y,z
C9-H9	0.94	2.58	3.485(3)	162	O1	x,1/2-y,-1/2+z
Complex **2**						
N5-H15a	0.81(5)	2.23(5)	2.601(5)	108(4)	N3	intra
N5-H15a	0.81(5)	2.82(5)	3.503(4)	144(4)	S1	x,1/2-y,-1/2+z
N5-H15b	0.71(5)	2.23(5)	2.919(5)	167(5)	N6	1+x,1/2-y,1/2+z
C3-H3	0.95	2.46	3.112(5)	126	O1	1+x,y,z
Complex **3**						
N5-H15a	0.71(4)	2.31(4)	2.589(4)	106(4)	N3	intra
N5-H15a	0.71(4)	2.46(4)	3.103(4)	153(4)	O2	1-x,-y,1-z
N5-H15b	0.82(4)	2.18(4)	2.945(4)	156(4)	N6	1-x,1/2+y,1/2-z
C2-H2	0.95	2.31	3.115(4)	142	O1	2-x,1/2+y,3/2-z
C10-H10	0.95	2.51	3.441(4)	167	O2	x,-1/2-y,-1/2+z
Complex **4**						
N5-H5a	0.84(9)	2.16(9)	2.561(9)	110(7)	N3	intra
N5-H5a	0.84(9)	2.53(10)	3.266(10)	147(8)	O2	1-x,-y,-z
N5-H5b	0.78(10)	2.26(0)	2.954(10)	149(8)	N6	1-x,-1/2+y,-1/2-z
C1-H1	0.94	2.53	3.250(12)	134	O3	2-x,-y,1-z
C2-H2	0.94	2.44	3.130(10)	131	O1	2-x,-1/2+y,1/2-z
C8-H8	0.94	2.58	3.302(9)	134	O2	1-x,-y,-z
C10-H10	0.94	2.60	3.138(12)	116	N5	1-x,1/2+y,-1/2-z
C10-H10	0.94	2.50	3.306(10)	144'	O2	x,1/2-y,-1/2+z

Table S3. π···stacking interaction distances (Å) and angles (°) for complexes **1** - **4** (py = pyridine N6, pz = pyrazine N1/N4).

Cg(I)	Cg(J)	Cg(J) Symmetry	d(Cg(I)-Cg(J)) Å	α/°	β/°	γ/°	Slippage Å
Complex **1**							
Pz	Pz	3-x, -y, 2-z	3.545(1)	0.00(9)	26.0	26.0	1.552
Pz	Py	2-x, -y, 1-z	3.562(1)	5.70(9)	21.8	26.0	1.322
Py	Pz	2-x, -y, 1-z	3.562(1)	5.70(9)	26.0	21.8	1.560
Complex **2**							
Pz	Py	-x, -y, 1-z	3.563(2)	0.45(17)	24.5	24.6	1.480
Py	Pz	-x, -y, 1-z	3.563(2)	0.45(17)	24.6	24.5	1.482
Complex **3**							
Pz	Py	1-x, -y, 1-z	3.560(2)	3.37(16)	20.1	19.3	1.226
Pz	Py	2-x, -y, 1-z	3.635(2)	3.37(16)	25.3	24.1	1.552
Py	Pz	1-x, -y, 1-z	3.560(2)	3.37(16)	19.3	20.1	1.175
Py	Pz	2-x, -y, 1-z	3.635(2)	3.37(16)	24.1	25.3	1.484
Complex **4**							
Pz	Py	1-x, -y, -z	3.585(5)	4.6(4)	15.2	15.2	0.940
Pz	Py	2-x, -y, -z	3.558(5)	4.6(4)	20.2	18.6	1.228
Py	Pz	1-x, -y, -z	3.585(5)	4.6(4)	15.2	15.2	0.939
Py	Pz	2-x, -y, -z	3.558(5)	4.6(4)	18.6	20.2	1.135