On the importance of tetrel bonding interactions in Lead(II) complexes with (iso)nicotinohydrazide based ligands and several anions

Ghodrat Mahmoudi,[a]* Antonio Bauzá,[b] Mojtaba Amini,[a] Elies Molins,[c] Joel T. Mague[d] and Antonio Frontera[b,]*

[a]*Department of Chemistry, Faculty of Science, University of Maragheh, P.O. Box 55181–83111, Maragheh, Iran. E–mail: mahmoudi_ghodrat@yahoo.co.uk*

[b]*Departamento de Quimica, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma de Mallorca (Baleares), Spain; E–mail: toni.frontera@uib.es*

[c]*Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus de la Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain*

[d]*Department of Chemistry, Tulane University, New Orleans, LA 70118, USA*

Table of contents:

1. Tables S1 to S4

Table S1. Selected bond lengths [Å] and bond angles [º] for (**1**)

Atom Labels	Distance/angle
Pb1 N1A	2.37(1)
Pb1 N1	2.712(9)
Pb1 N6	2.548(9)
Pb1 O7	2.370(8)
Pb1 N9	2.89(1)
N1A Pb1 N1	86.1(3)
N1A Pb1 N6	81.7(3)
N1A Pb1 O7	91.4(3)
N1A Pb1 N9	88.2(3)
N1 Pb1 N6	62.3(2)
N6 Pb1 O7	62.8(3)
O7 Pb1 N9	74.7(3)
N9 Pb1 N1	159.8(3)

Table S2. Selected bond lengths [Å] and bond angles [º] for (**2**)

Atom Labels	Distance/angle
O1 Pb1	2.521(3)
O2 Pb1	2.757(3)
O4 Pb1	2.867(2)
O6 Pb1	2.708(2)
O7 Pb1	2.511(3)
N1 Pb1	2.531(3)
N2 Pb1	2.637(2)
O4 Pb1 O2	70.90(8)
O4 Pb1 O1	119.12(8)
O4 Pb1 N1	87.23(8)
O4 Pb1 O7	149.79(8)
O4 Pb1 O6	104.51(8)
O6 Pb1 N1	87.05(8)
O6 Pb1 N2	63.55(8)
O6 Pb1 O7	73.44(8)
O1 Pb1 O2	48.46(8)
O1 Pb1 O6	132.45(8)
O7 Pb1 N2	61.12(8)
N2 Pb1 N1	61.48(8)

Table S3. Selected bond lengths [Å] and bond angles [º] for (**3**)

Atom Labels	**Distance/angle**
Pb1 O1	2.643(5)
Pb1 N2	2.693(5)
Pb1 N3	2.673(6)
Pb1 I1	2.9386(6)
Pb1 I2	3.1810(7)
O1 Pb1 N2	59.6(2)
O1 Pb1 N3	117.2(2)
O1 Pb1 I2	153.4(1)
O1 Pb1 I1	81.9(1)
N2 Pb1 N3	59.1(2)
N2 Pb1 I2	146.7(1)
N2 Pb1 I1	87.1(1)
N3 Pb1 I2	87.9(1)
N3 Pb1 I1	82.7(1)
I2 Pb1 I1	93.63(2)
1 O1 Pb1 O3 85.6(2)	
2 O1 Pb1 N1 82.5(2)	
3 O1 Pb1 N3 80.4(2)	
4 O3 Pb1 N1 65.4(2)	
5 O3 Pb1 N3 128.6(2)	
6 N1 Pb1 N3 63.9(2)	

Table S4. Selected bond lengths [Å] and bond angles [º] for (**4**)

Atom Labels	**Distance/angle**
Pb1 N1	2.462(7)
Pb1 N3	2.603(8)
Pb1 O1	2.277(7)
Pb1 O3	2.415(6)
O1 Pb1 O3	85.6(2)
O1 Pb1 N1	82.5(2)
O1 Pb1 N3	80.4(2)
O3 Pb1 N1	65.4(2)
O3 Pb1 N3	128.6(2)
N1 Pb1 N3	63.9(2)

2. Figs S1 to S3:

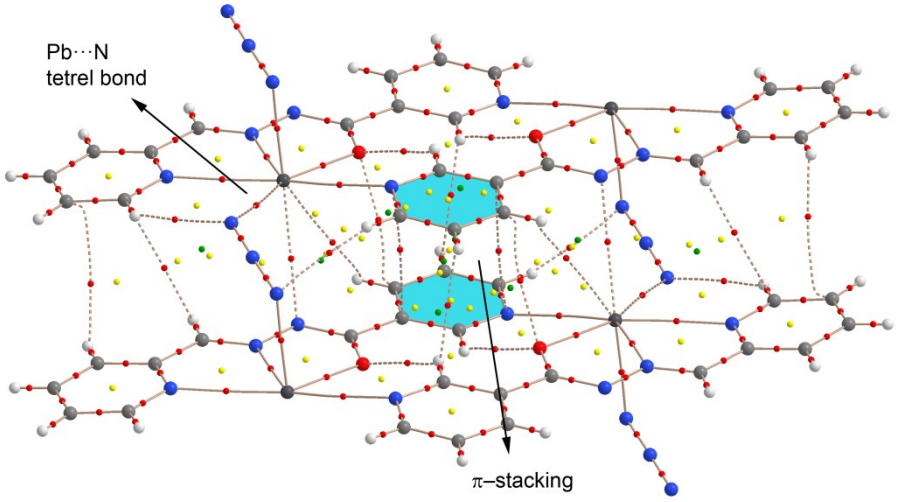

Fig. S1. AIM analysis of the dimer of complex **1**. Bond, ring and cage critical points are represented by red, yellow and green spheres, respectively. The bond paths connecting bond critical points are also represented by dashed lines.

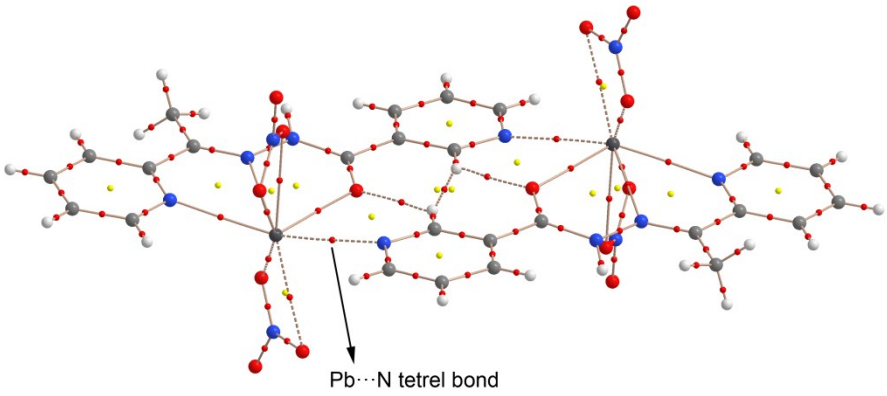

Fig. S2. AIM analysis of the dimer of complex **2**. Bond, ring and cage critical points are represented by red, yellow and green spheres, respectively. The bond paths connecting bond critical points are also represented by dashed lines.

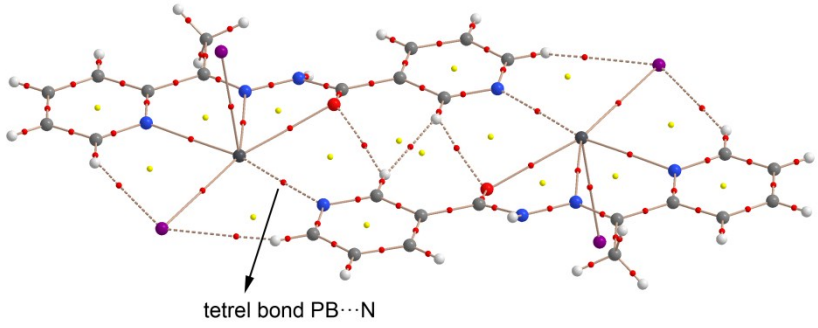

Fig. S3. AIM analysis of the dimer of complex **3**. Bond and ring critical points are represented by red and yellow spheres, respectively. The bond paths connecting bond critical points are also represented by dashed lines.