

Supporting Information

Bismuth-Lithium Bonding in the Iron Pairs: LiBiL_2 , Where L= a Porphyrin or a Salen Ligand

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Select bond distances and angles for **IIIA**, **IIIB**, and **IV**.

IIIA

Select Bond Distances – in ang.

Bi(1)-O(3)	2.224(2)
Bi(1)-O(4)	2.241(3)
Bi(1)-N(1)	2.381(3)
Bi(1)-N(2)	2.399(3)
Bi(1)-O(2)	2.467(2)
Bi(1)-O(1)	2.659(3)
Bi(1)-Li(1)	3.137(7)
Li(1)-O(1)	1.940(7)
Li(1)-O(2)	1.957(7)
Li(1)-N(4)	2.034(7)
Li(1)-N(3)	2.053(7)

Select Angles – in degrees.

O(3)-Bi(1)-O(4)	82.66(10)
O(3)-Bi(1)-N(1)	76.05(10)
O(4)-Bi(1)-N(1)	125.59(10)
O(3)-Bi(1)-N(2)	112.72(10)
O(4)-Bi(1)-N(2)	76.17(10)
N(1)-Bi(1)-N(2)	67.51(10)
O(3)-Bi(1)-O(2)	148.63(9)
O(4)-Bi(1)-O(2)	128.11(9)
N(1)-Bi(1)-O(2)	87.62(9)
N(2)-Bi(1)-O(2)	84.27(9)
O(3)-Bi(1)-O(1)	92.39(9)
O(4)-Bi(1)-O(1)	126.82(9)
N(1)-Bi(1)-O(1)	103.81(9)
N(2)-Bi(1)-O(1)	149.10(9)

O(2)-Bi(1)-O(1)	65.39(8)
O(3)-Bi(1)-Li(1)	110.57(13)
O(4)-Bi(1)-Li(1)	157.39(14)
N(1)-Bi(1)-Li(1)	76.42(14)
N(2)-Bi(1)-Li(1)	112.83(14)
O(2)-Bi(1)-Li(1)	38.58(13)
O(1)-Bi(1)-Li(1)	37.98(13)
O(1)-Li(1)-O(2)	90.8(3)
O(1)-Li(1)-N(4)	157.4(4)
O(2)-Li(1)-N(4)	89.0(3)
O(1)-Li(1)-N(3)	89.0(3)
O(2)-Li(1)-N(3)	149.9(4)
N(4)-Li(1)-N(3)	80.1(3)
O(1)-Li(1)-Bi(1)	57.53(18)
O(2)-Li(1)-Bi(1)	51.83(17)
N(4)-Li(1)-Bi(1)	106.0(3)
N(3)-Li(1)-Bi(1)	104.3(3)

IIIB

Select Bond Distances – in ang.

Bi(2)-O(2)	2.067(2)
Bi(2)-N(4)	2.313(3)
Bi(2)-O(1)	2.319(2)
Bi(2)-N(3)	2.552(3)
Bi(2)-O(4)	2.621(2)
Bi(2)-N(2)	2.720(3)
Bi(2)-Li(2)	3.005(18)
Li(2)-O(3)	2.00(2)
Li(2)-O(4)	2.038(18)
Li(2)-N(1)	2.261(18)
Li(2)-N(2)	2.384(19)

Select Angles – in degrees.

O4- Bi1- O3	78.41(9)
O4- Bi1- N2	75.09(9)
O3- Bi1- N2	113.69(10)
O4- Bi1- N1	111.56(10)
O3- Bi1- N1	71.68(9)
N2- Bi1- N1	64.16(9)
O4- Bi1- O2	93.81(8)
O3- Bi1- O2	111.35(8)

N2- Bi1- O2	129.89(8)
N1- Bi1- O2	154.31(9)
O4- Bi1- O1	156.48(8)
O3- Bi1- O1	102.86(8)
N2- Bi1- O1	123.69(8)
N1- Bi1- O1	90.73(8)
O2- Bi1- O1	63.59(7)
O4- Bi1- Li1	127.06(17)
O3- Bi1- Li1	135.49(19)
N2- Bi1- Li1	108.50(19)
N1- Bi1- Li1	117.15(17)
O2- Bi1- Li1	42.13(17)
O1- Bi1- Li1	38.44(17)
O1B- Li1- O1	120.2(5)
O1B- Li1- O2	116.9(5)
O1- Li1- O2	93.4(4)
O1B- Li1- N3	106.4(5)
O1- Li1- N3	84.7(3)
O2- Li1- N3	130.2(4)
O1B- Li1- N4	109.8(4)
O1- Li1- N4	128.2(4)
O2- Li1- N4	74.6(3)
N3- Li1- N4	68.4(3)
O1B- Li1- Bi1	173.9(5)
O1- Li1- Bi1	65.9(2)
O2- Li1- Bi1	60.6(2)
N3- Li1- Bi1	73.8(2)
N4- Li1- Bi1	64.4(2)

IV

Select Bond Distances – in ang.

Li(3)-O(6)	1.986(10)
Li(3)-O(5)	2.008(10)
Li(3)-N(3)	2.071(10)
Li(3)-N(4)	2.074(10)
Li(3)-Li(4)	2.465(15)
Li(4)-O(5)	1.792(10)
Li(4)-O(6)	1.824(11)

Li(1)-O(1)	1.984(11)
Li(1)-O(2)	2.019(11)
Li(1)-N(2)	2.063(11)
Li(1)-N(1)	2.095(11)
Li(1)-Li(2)	2.460(16)
Li(2)-O(1)	1.804(12)
Li(2)-O(2)	1.806(11)

Select Angles – in degrees.

C(1A)-O(8A)-Li(3)	127.3(11)
C(4A)-O(8A)-Li(3)	118.0(11)
C(12A)-O(3A)-Li(1)	123.6(10)
C(9A)-O(3A)-Li(1)	119.9(12)
C(13A)-O(4A)-Li(2)	122(4)
C(16A)-O(4A)-Li(2)	125.8(14)
C(5A)-O(7A)-Li(4)	121.7(13)
C(8A)-O(7A)-Li(4)	118.0(14)
O(8A)-Li(3)-O(6)	109.5(5)
O(8A)-Li(3)-O(5)	112.5(5)
O(6)-Li(3)-O(5)	87.3(4)
O(8A)-Li(3)-N(3)	100.6(5)
O(6)-Li(3)-N(3)	149.5(6)
O(5)-Li(3)-N(3)	85.7(4)
O(8A)-Li(3)-N(4)	105.8(5)
O(6)-Li(3)-N(4)	87.9(4)
O(5)-Li(3)-N(4)	140.8(6)
N(3)-Li(3)-N(4)	79.1(4)
O(8A)-Li(3)-Li(4)	137.2(6)
O(6)-Li(3)-Li(4)	46.9(3)
O(5)-Li(3)-Li(4)	45.8(3)
N(3)-Li(3)-Li(4)	111.3(5)
N(4)-Li(3)-Li(4)	107.6(5)
O(5)-Li(4)-O(6)	99.3(6)
O(5)-Li(4)-O(7A)	122.4(7)
O(6)-Li(4)-O(7A)	121.9(6)
O(5)-Li(4)-Li(3)	53.5(4)
O(6)-Li(4)-Li(3)	52.6(4)
O(7A)-Li(4)-Li(3)	123.4(6)
C(46)-N(3)-C(47)	122.0(4)

C(46)-N(3)-Li(3)	122.6(4)
C(47)-N(3)-Li(3)	112.8(4)
C(53)-N(4)-C(52)	121.9(4)
C(53)-N(4)-Li(3)	125.5(4)
C(52)-N(4)-Li(3)	112.4(4)
C(40)-O(5)-Li(4)	150.3(5)
C(40)-O(5)-Li(3)	126.3(4)
Li(4)-O(5)-Li(3)	80.6(5)
C(55)-O(6)-Li(4)	138.7(5)
C(55)-O(6)-Li(3)	127.6(4)
Li(4)-O(6)-Li(3)	80.5(5)