Supporting Information

Lipophilic Bismuth Phosphates: A Molecular Tetradecanuclear Cage and a 1D-Coordination Polymer. Synthesis, Structure and Conversion to BiPO_4

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Figure S1 ESI-MS of 1
$[(\text{Bi}(L_1\text{H})_2(\text{CH}_3\text{OH})_2)]^+$

**a) Experimental**

**b) Simulated**

**Figure S2** ESI-MS isotopic pattern of fragment in 1.
**Figure S3** $^{31}$P NMR spectra of 1
Figure S4. View showing the 3D arrangement in 1. Hydrogen atoms have been omitted for the sake of clarity.
Figure S5 ESI-MS of 2
Figure S6 ESI-MS isotopic pattern for the fragments in 2.
Figure S7 $^{31}$P NMR spectra of 2
Figure S8. View showing the 2D arrangement of the 1D polymeric chain in 2 resulting due to C-H…π interactions. The metric parameters involved are: C(10)-H(10), 0.930 (8)Å  C10-H10…π, 3.698 (8) Å, C10-H10…π, 130.68 (4)°; C(12)-H(12), 0.930 (7)Å, C12-H12…π, 4.271 (1) Å, C12-H12…π, 133.65 (4)°. Hydrogen atoms have been omitted for the sake of clarity.
**Chart S1:** Presence of Stereochemically active lone pair of bismuth atoms in 1 (green color) and 2 (blue color), the arrows show the approximate location of lone pair electrons.
Table S1. Individual coordination environment of bismuth in 1 and Selected bond lengths (Å) and bond angles (°) parameters.

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<tr>
<td>C(10)-C(11)</td>
<td>1.391(11)</td>
</tr>
</tbody>
</table>
C(13)-C(15)  1.509(11)
C(13)-C(16)  1.529(12)
C(13)-C(14)  1.539(13)
C(17)-C(18)  1.514(11)
C(17)-C(20)  1.521(11)
C(17)-C(19)  1.543(11)

C(1)-Bi(1)-C(7)  91.3(3)
C(1)-Bi(1)-O(4)  88.9(2)
C(7)-Bi(1)-O(4)  86.9(2)
C(1)-Bi(1)-O(1)  89.4(2)
C(7)-Bi(1)-O(1)  85.1(2)
O(4)-Bi(1)-O(1)  171.81(18)
O(1)-P(1)-O(4)#1  116.3(3)
O(1)-P(1)-O(3)  105.3(3)
O(4)#1-P(1)-O(3)  112.0(3)
O(1)-P(1)-O(2)  111.5(3)
O(4)#1-P(1)-O(2)  103.6(3)
O(3)-P(1)-O(2)  108.1(3)
P(1)-O(1)-Bi(1)  129.2(3)
C(13)-O(2)-P(1)  128.8(5)
C(17)-O(3)-P(1)  129.6(5)
P(1)#2-O(4)-Bi(1)  123.7(3)
C(2)-C(1)-C(6)  119.2(7)
C(2)-C(1)-Bi(1)  121.5(6)
C(6)-C(1)-Bi(1)  119.2(5)
C(1)-C(2)-C(3) 121.1(7)
C(2)-C(3)-C(4) 120.5(8)
C(3)-C(4)-C(5) 119.0(8)
C(6)-C(5)-C(4) 120.2(8)
C(5)-C(6)-C(1) 119.9(7)
C(8)-C(7)-C(11) 119.5(7)
C(8)-C(7)-Bi(1) 120.6(6)
C(11)-C(7)-Bi(1) 119.9(5)
C(7)-C(8)-C(12) 120.3(7)
C(10)-C(9)-C(12) 119.4(8)
C(9)-C(10)-C(11) 121.2(8)
C(10)-C(11)-C(7) 119.3(7)
C(8)-C(12)-C(9) 120.2(8)
O(2)-C(13)-C(15) 108.1(7)
O(2)-C(13)-C(16) 111.3(7)
C(15)-C(13)-C(16) 111.4(7)
O(2)-C(13)-C(14) 103.4(7)
C(15)-C(13)-C(14) 112.4(8)
C(16)-C(13)-C(14) 110.0(8)
O(3)-C(17)-C(18) 110.1(6)
O(3)-C(17)-C(20) 102.8(6)
C(18)-C(17)-C(20) 112.4(7)
O(3)-C(17)-C(19) 109.4(6)
C(18)-C(17)-C(19) 111.3(7)
C(20)-C(17)-C(19) 110.5(7)
Symmetry transformations used to generate equivalent atoms:

#1 x,-y+1/2,z-1/2    #2 x,-y+1/2,z+1/2