Supplementary Information for

Synthesis and characterisation of iodobismuthates containing N-substituted 1,4-diazabicyclo[2.2.2]octane

Yunhe Cai, Ann M. Chippindale and Paz Vaqueiro

Department of Chemistry, University of Reading, Whiteknights, Reading, Berkshire, RG6 6DX, United Kingdom

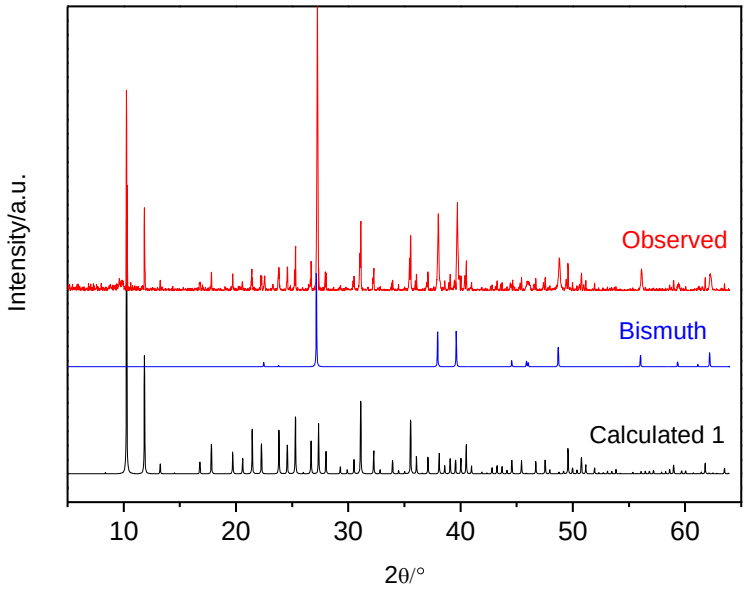

Figure S1. Powder diffraction pattern of the solid product of the reaction producing compound **1** (red line). The pattern calculated using the structure for **1,** determined by single-crystal X-ray diffraction, is shown in black and that calculated for bismuth metal is shown as a blue line.

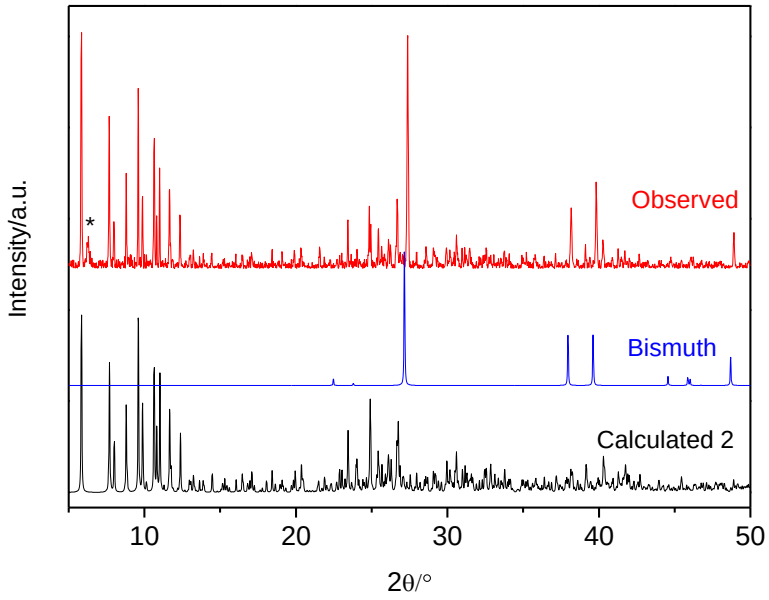

Figure S2. Powder diffraction pattern of the solid product of the reaction producing compound **2** (red line). The pattern calculated using the structure for **2,** determined by single-crystal X-ray diffraction, is shown in black and that calculated for bismuth metal is shown as a blue line. The asterisk marks peaks possibly arise from compound **3**.

Table S1. Lattice parameters of compounds **1** and **2** determined using powder X-ray diffraction data collected at room temperature.

Compound	**1**	**2**
a/Å	14.998(82)	8.970(2)
b/Å	14.998(82)	40.10(5)
c/Å	14.998(82)	22.97(5)
β/°	90	92.5(3)

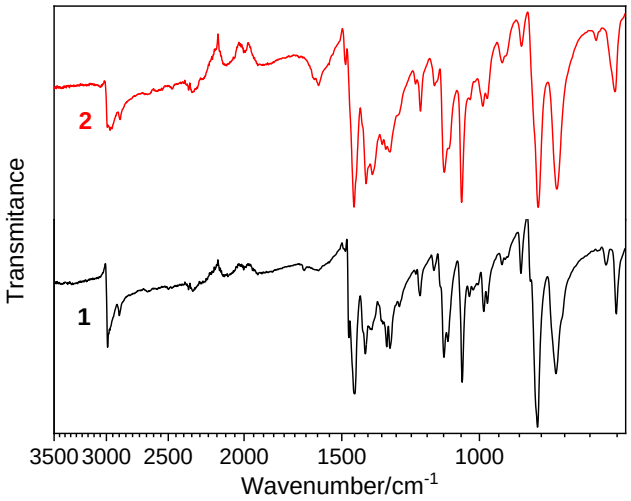

Figure S3. FTIR data collected on hand-picked single crystals of compounds **1** (black line) and **2** (red line).

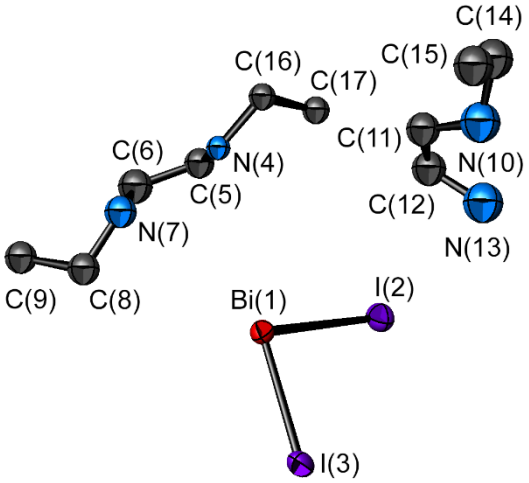

Figure S4. Asymmetric unit of compound **1** with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

Table S2 Short C-H···I contacts (Å) for compound **1.**

I(2)···H(111)^{i}	3.075(28)
I(2)···H(112)^{ii}	3.298(26)
I(2)···H(121)^{iii}	3.284(25)
I(2)···H(122)^{iv}	3.080(28)
I(2)···H(142)^{i}	3.118(2)
I(3)···H(51)^{v}	3.144(24)
I(3)···H(52)^{vi}	3.069(25)
I(3)···H(61)^{vii}	3.392(25)
I(3)···H(62)^{viii}	3.145(28)
I(3)···H(81)^{viii}	3.141(2)
I(3)···H(82)^{ix}	3.056(2)
I(3)···H(93)^{vii}	3.254(2)
I(3)···H(161)^{x}	3.384(2)
I(3)···H(172)^{vi}	3.374(2)

Symmetry codes: (i) 1/2 + *x*, 3/2 – *y*, 1 – *z*; (ii) z, 1 + *x*, *y*; (iii) *y* – 1/2, 3/2 – *z*, –*x*; (iv) –*x*, 1 + *y*, 1/2 – *z*; (v) 1 – *z*, *x* + 1/2, 1/2 – *y*; (vi) 1 – *y*, 1/2 + *z*, 1/2 – *x*; (vii) 1/2 – *x*, 1 – *y*, *z* – 1/2; (viii) 1/2 – *z*, 1 – *x*, *y* – 1/2; (ix) 1/2 – *y*, 1 – *x*, *z* – 1/2; (x) 1 – *x*, 1/2 + *y*, 1/2 – *z*.

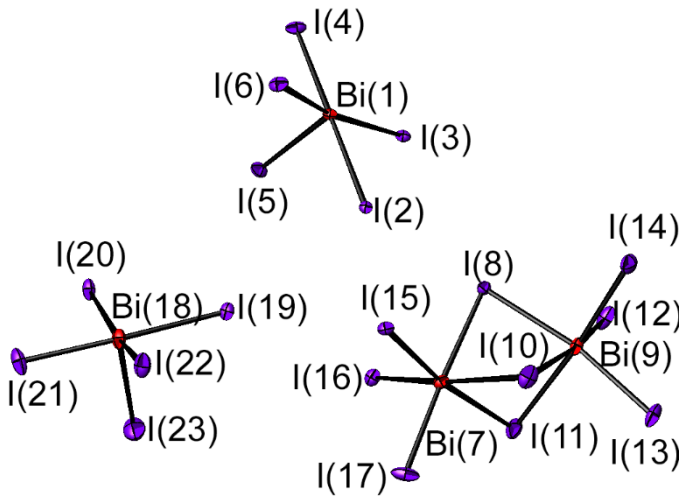

Figure S5. The inorganic anions in the asymmetric unit of compound **2** with displacement ellipsoids drawn at the 50% probability level.

Table S3 Short intermolecular I···I contacts (Å) for compound **2.**

I(2) ···I(8)	4.131(1)
I(4) ···I(5)	4.183(1)
I(4) ···I(8)^{i}	3.910(1)
I(5) ···I(21)^{ii}	4.187(1)
I(8) ···I(10)	4.166(1)
I(12) ···I(14)	4.176(1)
I(20) ···I(20)^{iii}	4.147(1)

Symmetry codes: (i) 1– *x*, 1 – *y*, 2 – *z*; (ii) 1 – *x*, 1 – *y*, 1 – *z*; (iii) 2 – *x*, 1 – *y*, 1 – *z*.