

Table 3. The coordination tables of cations. The bold numbers on the diagonals are the bond distances (Å), the numbers above the diagonal the bond angles (°), and the numbers below the diagonal the ligand – ligand distances.

Atom **Bi1**

	S1	S2	S2	I1	I1	I1	I1
S1	2.556 (5)	90.4 (1)	90.4 (1)	80.5 (1)	80.5 (1)	145.1 (1)	145.1 (1)
S2	3.704 (5)	2.664 (2)	100.8 (2)	163.6 (1)	92.9 (1)	122.6 (1)	73.6 (1)
S2	3.704 (5)	4.105 (1)	2.664 (2)	92.9 (1)	163.6 (1)	73.6 (1)	122.6 (1)
I1	3.964 (4)	6.084 (3)	4.490 (4)	3.482 (1)	72.2 (0)	69.9 (0)	106.5 (0)
I1	3.964 (4)	4.490 (4)	6.084 (3)	4.105 (1)	3.482 (1)	106.5 (0)	69.9 (0)
I1	6.125 (5)	5.743 (3)	4.016 (5)	4.212 (2)	5.881 (2)	3.852 (1)	64.4 (0)
I1	6.125 (5)	4.016 (5)	5.743 (3)	5.881 (2)	4.212 (2)	4.105 (1)	3.852 (1)

Atom **Bi2A**

	S3	S3	S3	I3	I3	I2	I2
S3	2.624 (6)	82.5 (2)	82.5 (2)	80.8 (1)	80.8 (1)	145.5 (1)	145.5 (1)
S3	3.534 (5)	2.735 (3)	97.2 (2)	161.6 (1)	88.2 (1)	74.0 (1)	124.7 (1)
S3	3.534 (5)	4.105 (1)	2.735 (3)	88.2 (1)	161.6 (1)	124.7 (1)	74.0 (1)
I3	3.756 (4)	5.800 (3)	4.097 (4)	3.140 (2)	81.6 (1)	117.1 (1)	73.7 (1)
I3	3.756 (4)	4.097 (4)	5.800 (3)	4.105 (1)	3.140 (2)	73.7 (1)	117.1 (1)
I2	5.994 (5)	3.907 (5)	5.667 (3)	5.794 (2)	4.089 (3)	3.644 (3)	68.6 (1)
I2	5.994 (5)	5.667 (3)	3.907 (5)	4.089 (3)	5.794 (2)	4.105 (1)	3.644 (3)

Atom **Bi2B**

	S3	S4	S4	S3	S3	I2	I2
S3	2.579 (8)	88.2 (2)	88.2 (2)	77.5 (2)	77.5 (2)	143.9 (2)	143.9 (2)
S4	3.756 (4)	2.811 (3)	93.8 (2)	165.4 (2)	88.9 (1)	124.6 (2)	76.2 (1)
S4	3.756 (4)	4.105 (1)	2.811 (3)	88.9 (1)	165.4 (2)	76.2 (1)	124.6 (2)

S3	3.534(5)	5.800(3)	4.097(4)	3.036(4)	85.1(2)	69.9(1)	113.8(2)
S3	3.534(5)	4.097(4)	5.800(3)	4.105(1)	3.036(4)	113.8(2)	69.9(1)
I2	5.994(5)	5.794(2)	4.089(3)	3.907(5)	5.667(3)	3.715(6)	67.1(1)
I2	5.994(5)	4.089(3)	5.794(2)	5.667(3)	3.907(5)	4.105(1)	3.715(6)

Atom **Cu1**

	S3	S1	I1	I1
S3	2.196(5)	140.3(2)	105.9(1)	105.9(1)
S1	4.185(5)	2.254(4)	101.3(1)	101.3(1)
I1	4.043(4)	3.964(4)	2.847(3)	92.3(1)
I1	4.043(4)	3.964(4)	4.105(1)	2.847(3)

Atom **Cu2A**

	S2	S1	S1	I3
S2	2.251(6)	115.8(2)	115.8(2)	85.1(1)
S1	3.839(5)	2.280(3)	128.3(2)	91.5(1)
S1	3.839(5)	4.105(1)	2.280(3)	91.5(1)
I3	3.633(4)	3.856(4)	3.856(4)	3.049(4)

Atom **Cu2B**

	S4	S1	S1	S2
S4	2.276(18)	115.6(6)	115.6(6)	83.6(4)
S1	3.856(4)	2.280(8)	128.4(6)	89.8(4)
S1	3.856(4)	4.105(1)	2.280(8)	89.8(4)
S2	3.633(4)	3.839(5)	3.839(5)	3.096(15)

Atom **Cu3**

	S2	S2	S1	S1
S2	2.521(7)	158.2(7)	99.1(5)	94.5(5)
S2	4.950(7)	2.521(7)	94.5(5)	99.1(5)

S1 3.839(5) 3.704(5) **2.525(16)** 102.7(5)

S1 3.704(5) 3.839(5) 3.944(5) **2.525(16)**

Atom **Cu4A**

	S4	S2	I2	I2
S4	2.157(10)	108.5(3)	115.3(3)	115.3(3)
S2	3.633(4)	2.318(9)	110.6(3)	110.6(3)
I2	4.169(2)	4.184(4)	2.762(8)	96.0(2)
I2	4.169(2)	4.184(4)	4.105(1)	2.762(8)

Atom **Cu4B**

	S2	I2	I2	I1
S2	2.294(12)	118.2(3)	118.2(3)	102.9(3)
I2	4.184(4)	2.578(5)	105.5(3)	105.2(3)
I2	4.184(4)	4.105(1)	2.578(5)	105.2(3)
I1	4.016(5)	4.295(1)	4.295(1)	2.823(10)

Atom **Cu4C**

	S2	I2	I2	I3	I1
S2	2.232(13)	123.3(5)	123.3(5)	89.9(4)	80.4(3)
I2	4.184(4)	2.521(8)	109.0(4)	101.1(4)	84.4(3)
I2	4.184(4)	4.105(1)	2.521(8)	101.1(4)	84.4(3)
I3	3.633(4)	4.169(2)	4.169(2)	2.872(15)	170.3(4)
I1	4.016(5)	4.295(1)	4.295(1)	6.579(2)	3.730(14)

Atom **Cu5**

	I3	I2	I2	I2
I3	2.518(18)	106.6(4)	107.7(4)	107.7(4)
I2	4.089(3)	2.583(12)	116.2(5)	116.2(5)
I2	4.169(2)	4.438(2)	2.643(9)	101.9(4)

I2 4.169(2) 4.438(2) 4.105(1) 2.643(9)