**Table 20A-1-001**. BiSCl. Structure [80Vou]. Fractional coordinates of atoms at RT.

| Atom | | |
|---|---|---|
| Bi | $x$ | 0.13966(4) |
| | $y$ | 0.13230(3) |
| | $z$ | 1/4 |
| S | $x$ | 0.8214(3) |
| | $y$ | 0.0486(2) |
| | $z$ | 1/4 |
| Cl | $x$ | 0.5194(3) |
| | $y$ | 0.8073(2) |
| | $z$ | 1/4 |

**Table 20A-1-002**. BiSCl. Structure [80Vou]. Anisotropic temperature parameters. $U_{ij}$ [Å$^2$] is defined by Eq. (d) in Introduction.

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{23}$ | $U_{13}$ |
|---|---|---|---|---|---|---|
| Bi | 0.0150(2) | 0.0138(2) | 0.0157(2) | –0.0022(1) | 0 | 0 |
| S | 0.0140(8) | 0.0124(7) | 0.0130(8) | –0.0012(6) | 0 | 0 |
| Cl | 0.0215(9) | 0.0169(9) | 0.0218(9) | –0.0037(7) | 0 | 0 |

**Table 20A-1-003**. BiSCl. Structure [80Vou]. Interatomic distances [Å] at RT. See Fig. 22A-1-002 for the numbers assigned to the atoms.

| | | | |
|---|---|---|---|
| Bi–Cl(1) | 2.927(2) Å | Cl(2)–Cl(3) | 4.041(4) Å |
| Cl(2) | 2.927(2) | S(1) | 3.492(3) |
| Cl(3) | 3.367(2) | S(2) | 3.873(3) |
| Cl(4) | 3.367(2) | | |
| S(1) | 2.605(2) | Cl(3)–Cl(4) | 3.996(0) |
| S(2) | 2.711(1) | S(2) | 3.360(3) |
| S(3) | 2.711(1) | | |
| | | Cl(4)–S(3) | 3.360(3) |
| Cl(1)–Cl(2) | 3.996(0) | S(1)–S(2) | 3.549(3) |
| Cl(4) | 4.041(4) | S(3) | 3.549(3) |
| S(1) | 3.492(3) | | |
| S(3) | 3.873(3) | S(2)–S(3) | 3.996(0) |

**Table 20A-1-004**. BiSCI. Bond angles [°] [80Vou]. See Fig. 20A-1-002 for the numbers assigned to the atoms.

| | | | |
|---|---|---|---|
| Cl(1)–Bi–Cl(2) | 86.08(5)° | Bi–Cl(1)–Cl(2) | 46.96(4)° |
| Cl(3) | 128.93(6) | Cl(4) | 55.03(4) |
| Cl(4) | 79.55(6) | S(1) | 46.86(4) |
| S(1) | 78.05(6) | S(2) | 44.33(3) |
| S(2) | 161.45(7) | | |
| S(3) | 86.68(5) | Bi–Cl(2)–Cl(3) | 55.03(4) |
| | | S(1) | 46.86(4) |
| Cl(2)–Bi–Cl(3) | 79.55(6) | S(2) | 44.33(3) |
| Cl(4) | 128.93(6) | | |
| S(1) | 78.05(6) | Bi–Cl(3)–Cl(2) | 45.43(4) |
| S(2) | 86.68(5) | Cl(4) | 53.61(4) |
| S(3) | 161.45(7) | S(2) | 47.52(4) |
| | | | |
| Cl(3)–Bi–Cl(4) | 72.79(4) | Bi–Cl(4)–Cl(1) | 45.43(4) |
| S(1) | 143.20(3) | Cl(3) | 53.61(4) |
| S(2) | 66.11(6) | S(3) | 47.52(4) |
| S(3) | 118.01(6) | | |
| | | Bi–S(1)–Cl(1) | 55.09(5) |
| Cl(4)–Bi–S(1) | 143.20(3) | Cl(2) | 55.09(5) |
| S(2) | 118.01(6) | S(2) | 49.40(4) |
| S(3) | 66.11(6) | S(3) | 49.40(4) |
| | | | |
| S(1)–Bi–S(2) | 83.75(6) | Bi–S(2)–Cl(2) | 48.99(4) |
| S(3) | 83.75(6) | Cl(3) | 66.37(5) |
| | | S(1) | 46.85(4) |
| S(2)–Bi–S(3) | 94.96(5) | S(3) | 42.52(3) |
| | | | |
| | | Bi–S(3)–Cl(1) | 48.99(4) |
| | | Cl(4) | 66.37(5) |
| | | S(1) | 46.85(4) |
| | | S(2) | 42.52(3) |