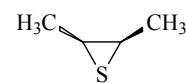


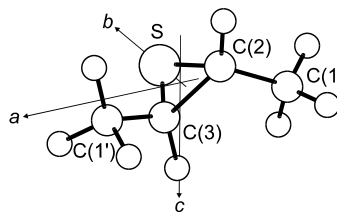
568
MW $\text{C}_4\text{H}_8\text{S}$ *trans*-2,3-Dimethylthiirane C_2 (see comment)

| r_0 | Å | θ_0 | deg |
|-----------|---------------------|------------------------------------|--------------------------|
| C(2)–C(3) | 1.487(9) | C(1)–C(2)–C(3) | 120.93(13) |
| C(2)–S | 1.830(3) | C(1)–C(2)–S | 118.02(32) ^{b)} |
| C(1)–C(2) | 1.509(6) | S–C(2)–C(3) | 66.02(13) ^{b)} |
| C(2)–H | 1.078 ^{a)} | C(2)–S–C(3) | 47.96(25) ^{b)} |
| C(1)–H | 1.09 ^{a)} | C(3)–C(2)–H | 117.80 ^{a)} |
| | | S–C(2)–H | 114.72 ^{a)} |
| | | C(2)–C(1)–H | 109.4 ^{a)} |
| | | C(1)–C(2)–C(3)–S ^{c)} | 109.44(20) |
| | | C(1)–C(2)–C(3)–C(1') ^{c)} | 141.12(40) ^{b)} |
| | | S–C(3)–C(2)–H ^{c)} | 106.50 ^{a)} |
| | | C(3)–C(2)–C(1)–H ^{c)} | 0.0 ^{a)} |

| r_s | Å | θ_s | deg |
|-----------|----------|------------------------------------|------------|
| C(2)–C(3) | 1.467(2) | C(1)–C(2)–C(3) | 120.70(30) |
| C(2)–S | 1.822(2) | C(1)–C(2)–S | 117.83(17) |
| C(1)–C(2) | 1.514(3) | S–C(2)–C(3) | 66.26(10) |
| | | C(2)–S–C(3) | 47.49(7) |
| | | C(1)–C(2)–C(3)–S ^{c)} | 109.39(17) |
| | | C(1)–C(2)–C(3)–C(1') ^{c)} | 141.23(19) |

| Atom | a_s [Å] | b_s [Å] | c_s [Å] |
|-------|-----------|-----------|-----------|
| C(2) | –0.5918 | –0.4443 | –0.4336 |
| C(3) | 0.5918 | –0.4443 | 0.4336 |
| C(1) | –1.9410 | –0.8765 | 0.1007 |
| C(1') | 1.9410 | –0.8765 | –0.1007 |
| S | 0.0 | 1.2233 | 0.0 |

G_{18} symmetry group applies when the internal rotation of two CH_3 groups is taken into account. Local C_{3v} symmetry was assumed for CH_3 group. The internal-rotation potential parameters are $V_3 = 13.1678(21)$ and $V_{12}' = -1.6678(25) \text{ kJ mol}^{-1}$.

^{a)} Assumed.^{b)} Dependent parameter.^{c)} Dihedral angle.

Hartwig, H., Dreizler, H.: Z. Naturforsch. A **51** (1996) 1099.