

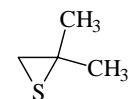
1766
MW

C₄H₈S

2,2-Dimethylthiirane

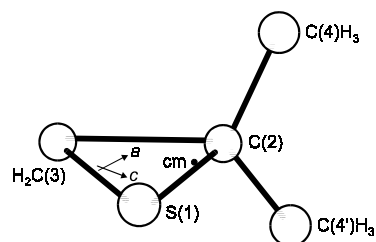
C_s

| r_0 | Å | θ_0 | deg |
|-----------|-----------|-----------------|----------|
| C(2)–C(3) | 1.513(10) | C(3)–C(2)–C(4) | 116.8(5) |
| S–C(3) | 1.821(7) | C(4)–C(2)–C(4') | 116.3(5) |
| S–C(2) | 1.838(2) | S–C(2)–C(4) | 116.0(4) |
| C(2)–C(4) | 1.509(4) | S–C(3)–C(2) | 66.2(4) |
| | | S–C(2)–C(3) | 65.0(3) |



| r_s | Å | θ_s | deg |
|-----------|-------|-----------------|-------|
| C(2)–C(3) | 1.478 | C(3)–C(2)–C(4) | 117.8 |
| S–C(3) | 1.822 | C(4)–C(2)–C(4') | 114.4 |
| S–C(2) | 1.820 | S–C(2)–C(4) | 116.2 |
| C(2)–C(4) | 1.518 | S–C(3)–C(2) | 66.0 |
| | | S–C(2)–C(3) | 66.1 |

| Atom | a_s [Å] | b_s [Å] | c_s [Å] |
|---------|-----------|-----------|-----------|
| C(3) | –0.4290 | [0.0] | 1.2258 |
| C(2) | 0.5092 | [0.0] | –0.0845 |
| C(4,4') | 1.2826 | ±1.2763 | 0.1950 |
| S | –1.2438 | [0.0] | –0.4035 |



Hartwig, H., Dreizler, H.: Z. Naturforsch. A **48** (1993) 1102.