

1150
MW

C₃H₄F₂

1,1-Difluorocyclopropane -*d*₄

C_{2v}

| r_0 | Å ^{a)} | θ_0 | deg ^{a)} |
|------------|-----------------|-------------------------|-------------------|
| C(1)–C(2) | 1.464(4) | F–C–F | 108.3(4) |
| C(2)–C(2') | 1.553(2) | C(2)–C(1)–C(2') | 64.1(2) |
| C–F | 1.355(4) | D–C–D | 116.9(4) |
| C–D | 1.082(4) | φ ^{b)} | 150.5(4) |

| Atom | x [Å] | y [Å] | z [Å] |
|-------|---------|---------|---------|
| F(1) | 1.0989 | 0.000 | 0.9388 |
| F(2) | –1.0989 | 0.000 | 0.9388 |
| C(1) | 0.000 | 0.000 | 0.1424 |
| C(2) | 0.000 | 0.7763 | –1.0959 |
| C(2') | 0.000 | –0.7763 | –1.0959 |
| D(1) | 0.9226 | 1.2694 | –1.3749 |
| D(2) | –0.9226 | 1.2694 | –1.3749 |
| D(3) | 0.9226 | –1.2694 | –1.3749 |
| D(4) | –0.9226 | –1.2694 | –1.3749 |

^{a)} Uncertainties are about twice those of the original paper.

^{b)} Angle between the plane DCD and the bond C(2)–C(2').

Perretta, A.T., Laurie, V.W.: J. Chem. Phys. **62** (1975) 2469.

