

1528
MW

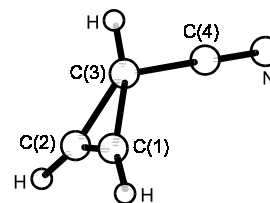
C₄H₃N

3-Cyanocyclopropene

C_s

| r_s | Å ^{a)} | θ_s | deg ^{a)} |
|-------------|-----------------|-------------------------|-------------------|
| C(1,2)–C(3) | 1.511(5) | H–C(1)=C(2) | 152.3(3) |
| C(1)=C(2) | 1.292(3) | H–C(3)–C(4) | 114.2(6) |
| C(3)–C(4) | 1.453(6) | φ ^{a)} | 122.9(6) |
| C(4)≡N | 1.162(5) | | |
| C(3)–H | 1.092(3) | | |
| C(1,2)–H | 1.071(4) | | |

| Atom | a_s [Å] | b_s [Å] | c_s [Å] |
|------|-----------|-----------|-----------|
| H(3) | 0.4246 | 0.0 | 1.6927 |
| H(1) | 1.8143 | 1.5942 | –0.5331 |
| C(4) | –1.0326 | 0.0 | 0.118 |



^{a)} Angle between the C(4)–C(3) bond and the ring plane.

Staley, S.W., Norden, T.D., Su, C.-F., Rall, M., Harmony, M.D.: J. Am. Chem. Soc. **109** (1987) 2880.