

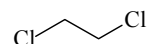
264
MW $C_2H_4Cl_2$

1,2-Dichloroethane

 C_2 (*gauche*)

| r_s | Å |
|----------------------|----------|
| C–C | 1.491(2) |
| C–Cl | 1.788(1) |
| C–H(a) ^{a)} | 1.108(2) |
| C–H(b) ^{a)} | 1.099(1) |

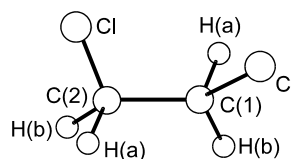
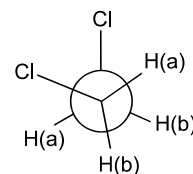
| θ_s | deg |
|---------------------------|----------|
| C–C–Cl | 112.1(2) |
| C–C–H(a) ^{a)} | 107.4(3) |
| C–C–H(b) ^{a)} | 111.3(1) |
| Cl–C–H(a) ^{a)} | 109.6(3) |
| Cl–C–H(b) ^{a)} | 105.7(1) |
| H(a)–C–H(b) ^{a)} | 110.8(3) |
| Cl–C–C–Cl ^{b)} | 68.3(4) |



| r_0 | Å |
|----------------------|-----------|
| C–C | 1.494(12) |
| C–Cl | 1.790(5) |
| C–H(a) ^{a)} | 1.108(9) |
| C–H(b) ^{a)} | 1.096(12) |

| θ_0 | deg |
|-------------------------|-----------|
| C–C–Cl | 112.2(1) |
| C–C–H(a) ^{a)} | 107.5(12) |
| C–C–H(b) ^{a)} | 111.5(16) |
| Cl–C–H(a) | 109.2(8) |
| Cl–C–H(b) | 105.6(10) |
| H(a)–C–H(b) | 110.8(25) |
| Cl–C–C–Cl ^{b)} | 67.9(4) |

| Atom ^{a)} | a_s [Å] | b_s [Å] | c_s [Å] |
|--------------------|-----------|-----------|-----------|
| Cl | ±1.6947 | 0.4113 | 0.0621 |
| C | ±0.6379 | −0.9597 | ±0.3855 |
| H(a) ^{c)} | ±0.3763 | −0.8916 | ±1.4596 |
| H(b) ^{d)} | ±1.2260 | −1.8657 | ±0.1836 |

^{a)} See figure for the definition of atoms.^{b)} Dihedral angle.^{c)} *Gauche* to Cl.^{d)} *Anti* to Cl.Sugie, M., Kato, M., Matsumura, C., Takeo, H.: J. Mol. Struct. **413-414** (1997) 487.[II/25B\(3, 737\)](#)