

1159  
MW

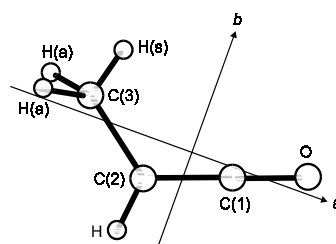
**C<sub>3</sub>H<sub>4</sub>O**

**1-Propen-1-one**  
Methylketene

**C<sub>s</sub>**  
H3C-CH=C=O

| $r_s$     | Å         | $\theta_s$                            | deg                    |
|-----------|-----------|---------------------------------------|------------------------|
| O=C(1)    | 1.171(5)  | O=C(1)=C(2)                           | 180.5(5) <sup>a)</sup> |
| C(1)=C(2) | 1.306(15) | C(1)=C(2)-C(3)                        | 122.6(3)               |
| C(2)-C(3) | 1.518(5)  | C(1)=C(2)-H                           | 113.7(5)               |
| C(2)-H    | 1.083(10) | C(3)-C(2)-H                           | 123.7(5)               |
| C(3)-H(s) | 1.083(10) | C(2)-C(3)-H(s)                        | 111.1(5)               |
|           |           | H-C(3)-H                              | 108.8(30)              |
|           |           | tilt (CH <sub>3</sub> ) <sup>b)</sup> | 2 <sup>c)</sup>        |

| Atom | $a_s$ [Å] | $b_s$ [Å] | $c_s$ [Å]   |
|------|-----------|-----------|-------------|
| O    | 1.7451    | 0.2460    | 0.00        |
| C(1) | 0.6414    | -0.1467   | 0.00        |
| C(2) | -0.5935   | -0.5730   | 0.00        |
| H    | -0.6813   | -1.6520   | 0.00        |
| C(3) | -1.7831   | 0.3694    | 0.00        |
| H(s) | -1.415    | 1.419     | 0.00        |
| H(a) | -2.411    | 0.21      | $\pm 0.904$ |



One of the C-H bonds is eclipsed with the C=C bond.

<sup>a)</sup> No definition of this angle was given in the original paper; the angle exceeding 180° probably means that the O atom is bent away from C(3).

<sup>b)</sup> Methyl tilt angle, defined positive if it is bent away from the C(1)=C(2) bond.

<sup>c)</sup> Assumed.

Bak, B., Christiansen, J.J., Kunstmann, K., Nygaard, L., Rastrup-Andersen, J.:  
J. Chem. Phys. **45** (1966) 883.