

1568  
MW

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

**2,4-Dioxabicyclo[3.1.0]hexan-3-one**

**C<sub>s</sub>**

| $r_s$      | Å                   | $\theta_s$      | deg               |
|------------|---------------------|-----------------|-------------------|
| C(1)–C(6)  | 1.522(15)           | C(1)–C(5)–C(6)  | 60.5(16)          |
| C(5)–C(6)  | 1.522(15)           | C(6)–C(1)–C(5)  | 60.5(16)          |
| C(1)–C(5)  | 1.497(16)           | C(1)–C(6)–C(5)  | 58.9(18)          |
| C(1)–H(1)  | 1.058 <sup>a)</sup> | H(6)–C(6)–H(6') | 116 <sup>b)</sup> |
| C(5)–H(5)  | 1.058 <sup>a)</sup> |                 |                   |
| C(3)=O(3)  | 1.191 <sup>a)</sup> |                 |                   |
| C(6)–H(6)  | 1.092 <sup>a)</sup> |                 |                   |
| C(6)–H(6') | 1.092 <sup>a)</sup> |                 |                   |
| O(2)–C(3)  | 1.364 <sup>a)</sup> |                 |                   |

| $r_0$     | Å <sup>c)</sup> | $\theta_0$     | deg <sup>c)</sup> |
|-----------|-----------------|----------------|-------------------|
| C(1)–O(2) | 1.408(12)       | C(5)–C(1)–O(2) | 105.80(6)         |
|           |                 | C(1)–O(2)–C(3) | 108.10(9)         |
|           |                 | O(2)–C(3)–O(4) | 112.18(6)         |
|           |                 | $\beta$        | 68.53(12)         |

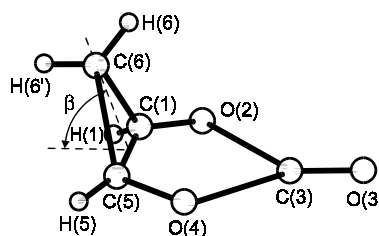
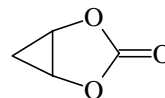
| Atom | $a_s$ [Å] | $b_s$ [Å]    | $c_s$ [Å] |
|------|-----------|--------------|-----------|
| C(6) | 1.7645    | 0.0          | 0.7590    |
| C(1) | 1.0893    | $\pm 0.7487$ | $-0.3815$ |

C(1)–H(1), C(5)–H(5) make an angle of 58° to the bisector C(6)–C(1)–C(5) = C(6)–C(5)–C(1) and in a plane orthogonal to C(6)–C(1)–C(5).

<sup>a)</sup> Assumed.

<sup>b)</sup> Bisected by C(1)–C(6)–C(5) plane.

<sup>c)</sup> Uncertainties are about three times those of the original data.



Bomar, S., Bay, E., Kraft, H.-G., Bevan, J. W.: J. Mol. Spectrosc. **87** (1981) 482.