

1705  
ED

**C<sub>4</sub>H<sub>7</sub>NO**

**Isopropyl isocyanate**

**C<sub>1</sub> (*skew*)**  
O=C=N-CH(CH<sub>3</sub>)<sub>2</sub>

| $r_a$    | Å <sup>a)</sup>    | $\theta_a$                  | deg <sup>a)</sup>    |
|----------|--------------------|-----------------------------|----------------------|
| C-N      | 1.460(8)           | N-C-C                       | 110.0(5)             |
| C-C      | 1.534(5)           | C-C-C                       | 114.7(9)             |
| N=C      | 1.214(6)           | C-N=C                       | 132.6(10)            |
| C=O      | 1.184(4)           | N=C=O                       | 159(3) <sup>b)</sup> |
| C(1,3)-H | 1.114(5)           | C(2)-C-H                    | 107 <sup>c)</sup>    |
| C(2)-H   | 1.09 <sup>c)</sup> | N-C-H                       | 105 <sup>c)</sup>    |
|          |                    | C(1)-C(2)-N=C <sup>d)</sup> | 125(3)               |

The data are consistent with the presence of a single *skew* conformer. The structure was consistent with the limited information available from microwave studies.

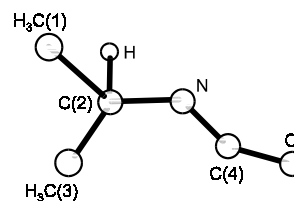
It was assumed that the two CH<sub>3</sub> groups were identical with local C<sub>3v</sub> symmetry about the C-C bonds, and that the N and unique H atoms were in the plane bisecting the C-C-C angle. The measurements were made at room temperature.

<sup>a)</sup> Unidentified, possibly estimated standard errors.

<sup>b)</sup> The C=O bond was assumed to be coplanar with the C(3)-C-N=C atoms and *trans* to the C(2)-N bond.

<sup>c)</sup> Assumed.

<sup>d)</sup> Zero position for the *syn* conformation.



Cradock, S., Sullivan, J.F., Durig, J.R.: J. Mol. Struct. **140** (1986) 199.