

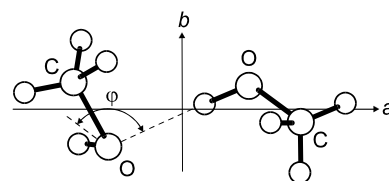
|                  |  |   |   |
|------------------|--|---|---|
| <b>313</b><br>MW | <b>C<sub>2</sub>H<sub>8</sub>O<sub>2</sub></b> | <b>Methanol dimer</b><br>(weakly bound complex) | <b>C<sub>1</sub></b><br>(large-amplitude motion)<br>CH <sub>3</sub> OH · CH <sub>3</sub> OH |
| $r_0$            | $\text{\AA}^a$                                 | $\theta_0$                                      | $\text{deg}^a$  |
| O...H            | 1.96(2)  | $\varphi^b$                                     | 77(2)   |
|                  |  | donor( <i>i,a</i> ) <sup>c</sup>                | 49.7(3)   |
|                  |  | donor( <i>i,b</i> ) <sup>c</sup>                | 110.5(18)   |
|                  |  | donor( <i>i,c</i> ) <sup>c</sup>                | 47.4(14)  |
|                  |  | acceptor( <i>i,a</i> ) <sup>c</sup>             | 120.79(2)   |
|                  |  | acceptor( <i>i,b</i> ) <sup>c</sup>             | 37.1(13)  |
|                  |  | acceptor( <i>i,c</i> ) <sup>c</sup>             | 71.4(20)  |

It was shown that the  $K = 1$  states are split into the 16 expected states through the assignment of the  $K_a = 1$   $a$ -type transitions and  $\Delta K_a = 1$   $b$ -type transitions. The effective barrier to internal rotation for the donor methyl group is  $V_3 = 183.0 \text{ cm}^{-1}$ , while the barrier to internal rotation of the acceptor methyl group is  $120 \text{ cm}^{-1}$ .

<sup>a</sup>) Estimated standard errors.

<sup>b</sup>) Tilt angle of the acceptor methanol defined by the O – H...O axis and the bisector of the H–O–C angle of the acceptor methanol. It was assumed that the donor proton is bonded symmetrically to the H–O–C angle.

<sup>c</sup>) Angle between the CH<sub>3</sub> internal rotation axis and the  $g$  ( $=a, b, c$ ) principal inertial axis.



Lovas, F.J., Hartwig, H.: J. Mol. Spectrosc. **185** (1997) 98.

Replaces [II/25B\(3, 942\)](#)