CO-DME

Analysis of Fourier transform microwave spectra of CO-dimethyl ether

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The tunneling–rotational spectra of the complex composed of CO and dimethyl ether (DME) measured by means of Fourier transform microwave spectroscopy have been analyzed for three isotope species of CO-DME, ^{13}CO-DME and C^{18}O-DME using a tunneling matrix formalism. Rotational constants and various tunneling parameters for these three isotopomers were determined in the present least squares analyses, where the large tunneling splitting caused by internal rotation of CO about the symmetry axis of DME and the small splittings by internal rotation of the methyl groups were treated simultaneously.

CO-dimethyl ether (CO-DME)

CO-DME Ar-DME Ne-DME [1]

DME

CO-DME

3.7~25.5 GHz CO-DME

^{13}CO-DME C^{18}O-DME

(i) DME CO

(ii) – C_s

36 G_{36}

(iii) tunneling

matrix method 1-1 dimethylsilacyclobutane(DMSCB)

[2]

$$H = h_v + AJ_z^2 + BJ_x^2 + CJ_y^2 + iq_zJ_z + iq_yJ_y +$$

h_v, A, B, C, q_z, q_y

$iq_z J_z + iq_y J_y$ Coriolis

$\langle 1|A|1\rangle$, $\langle 1|A|2\rangle$,... non-tunneling tunneling matrix element

(iv) a-type $K_a = 0 \leftarrow 0,\ 1 \leftarrow 1,\ 2 \leftarrow 2,\ 3 \leftarrow 3$; $J = 1 \leftarrow 0,\ 2 \leftarrow 1,\ 3 \leftarrow 2,\ 4 \leftarrow 3,\ 5 \leftarrow 4,\ 6 \leftarrow 5,\ 7 \leftarrow 6$ CO-DME, ^{13}CO-DME, C^{18}O-DME CO

$A_1 \leftrightarrow A_2$, $B_1 \leftrightarrow B_2$, $E_1 \leftrightarrow E_2$, $E_3 \leftarrow E_3$, $E_4 \leftarrow E_4$, $G \leftarrow G$

$A_1 \leftrightarrow A_2$, $B_1 \leftrightarrow B_2$ $K_a = 3 \leftarrow 3$, $J = 4 \leftarrow 3,\ 5 \leftarrow 4$ $E_3 \leftarrow E_3$, $E_4 \leftarrow E_4$, $G \leftarrow G$ E_1, E_2, E_3, E_4 E G E

(v) (root mean square deviation)

CO-DME 262 , 24 , = 3.7kHz

^{13}CO-DME 209 , 24 , = 3.8kHz

C^{18}O-DME 202 , 23 , = 3.9kHz

MHz

1σ $\langle 1|A|1\rangle$, $\langle 1|B|1\rangle$, $\langle 1|C|1\rangle$ $\langle 1|A|2\rangle$ CO $\langle 1|B|3\rangle$, $\langle 1|q_z|3\rangle$

	CO-DME	^{13}CO-DME	C^{18}O-DME
$\langle 1\|A\|1\rangle$	8792.35(8)	8738.2(1)	8732.4(1)
$\langle 1\|B\|1\rangle$	2025.8696(3)	1989.4955(4)	1937.9789(4)
$\langle 1\|C\|1\rangle$	1674.8282(2)	1648.258(3)	1612.1029(3)
$\langle 1\|h_v\|2\rangle$	-0.915(fixed)	-0.915(fixed)	-0.915(fixed)
$\langle 1\|A\|2\rangle$	9.80(3)	8.59(5)	8.58(5)
$\langle 1\|B\|2\rangle$	0.2435(3)	0.1927(3)	0.1849(3)
$\langle 1\|C\|2\rangle$	0.6177(3)	0.5440(3)	0.4190(2)
$\langle 1\|q_y\|2\rangle$	9.90(5)	8.60(7)	6.96(9)
$\langle 1\|B\|3\rangle$	0.00098(2)	0.00102(3)	0.00097(3)
$\langle 1\|q_z\|3\rangle$	0.1197(1)	0.117(1)	0.1164(9)

Fit CO $\langle 1|h_v|2\rangle$ $2|\langle 1|h_v|2\rangle|$ *ab initio*

CO-DME $\langle 1|q_z|3\rangle$ 779 cm^{-1} Ar-DME DME 85%

[1] Y. Morita, N. Ohashi, Y. Kawashima, E. Hirota, J. Chem. Phys. **124**, 094301-14 (2006).

[2] E. Hirota, N. Ohashi, Y. Kawashima, T. Usami, J. Mol. Spectrosc. **228**, 258-278 (2004).