CALCULATION OF MOLECULAR PARAMETERS FOR ISOTOPOMERS OF CD_3OH SPECIES OF METHANOL

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Tortion-rotational constants have been determined for ^{12}C and ^{13}C isotopomers of the CD_3OH species of methanol with O-16, 17 and 18, using the calculation procedure based on the centrifugal distortion theory for a molecule containing a three-fold symmetric internal rotor.[a] These parameters have also been obtained by fitting to obseved microwave lines[b] for $^{12}CD_3^{16}OH$ in which a correction-free reduced Hamiltonian[c] has been used. It is shown that all of the calculated constants are in better agreement with the fitting ones for this molecule than those for the other species of methanol.

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[b] M. S. Walsh, Li-Hong Xu, and R. M. Lees, J. Mol. Spectrosc. 188, 85 (1998); A. Predoi-Cross, Li-Hong Xu, M. S. Walsh, R. M. Lees, M. Winnerwisser, and H. Lichau, J. Mol. Spectrosc. 188, 94 (1998).

[c] Y. B. Duan, L. Wang, I. Mukhopadhyay, and K. Takagi, J. Chem. Phys. 110, 929 (1999).