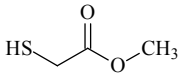
406 **$C_3H_6O_2S$** **Methyl mercaptoacetate** **C_s**
MW Mercaptoacetic acid methyl ester (effective symmetry class)
(large-amplitude motion)



Doublings due to two large-amplitude motions were observed and analyzed. The double-minimum potential associated with the SH group torsion generates a vibrational spacing Δ_{01} = 18953.0(7) MHz between the 0^+ and 0^- states of the A sublevel. The spacings between the E and A levels related to the methyl group internal rotation are Δ_{AE} = 295(2) and 291(3) MHz for the 0^+ and 0^- states, respectively. Both the thiolic hydrogen and the sulfur atom are largely out of the plane which contains all the remaining heavy atoms. The corresponding vibrational spacing for the SD group torsion in CH_3OCOCH_2SD, Δ_{01} = 8285(5) MHz, suggests a large involvement of the sulfur atom in the motion.

Fantoni, A.C., Caminati, W., Favero, P.G.: J. Mol. Spectrosc. **176** (1996) 364.
Maccaferri, G., Caminati, W., Favero, P.G., Fantoni, A.C.: J. Mol. Spectrosc. **186** (1997) 171.