

Structure Data of Free Polyatomic Molecules

136 IR	CH₆	Methane – dihydrogen (1/1) (weakly bound complex)	C_{3v} (effective symmetry class) (large-amplitude motion) CH ₄ · H ₂
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$$\frac{r_0}{R_{\text{cm}}} \text{ \AA}^{\text{a)}} = 4.12(3)$$

The structure of the *para* species was determined from the rovibrational spectrum in the ν_4 CH₄ fundamental region. The geometries of the monomer subunits were assumed to be unchanged upon complexation.

^{a)} Uncertainty was not estimated in the original paper.

McKellar, A.R.W., Roth, D.A., Pak, I., Winniewisser, G.: J. Chem. Phys. **110** (1999) 9989.