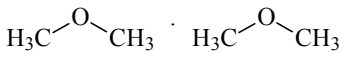
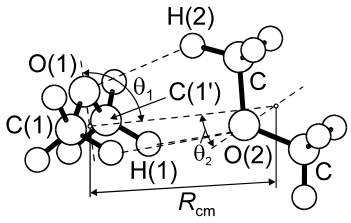
606 **$C_4H_{12}O_2$** **Dimethyl ether dimer** **C_s**

MW, *ab initio* calculations | Oxybismethane dimer (weakly bound complex) | (effective symmetry class) (large-amplitude motion)



r_0	Å [a])	θ_0	deg [a])
R_{cm}	3.80(1)	O(1)...H(2)–C	143.5(10)
C(1)...C(1') [b])	2.341(5)	θ_1 [c])	99.5(10)
O(1)...H(2)	2.53(2)	θ_2 [c])	35.0(10)
H(1)...O(2)	2.65(2)		

Two monomers are bound by three weak C–H...O hydrogen bonds, each with an average interaction energy of *ca.* 1.9 kJ mol^{-1}. The experimental data combined with high-level *ab initio* calculations show that this interaction is unusually blue-shifted hydrogen bonding, with an average shortening of the C–H bonds involved in the hydrogen bonding of 0.0014 Å. The length of the C–H...O hydrogen bonds, r(O...H) is in the range of 2.52 – 2.59 Å. The intermolecular stretching force constant and frequency are 4.7 N m^{-1} and 59 cm^{-1}, respectively, and the dissociation energy is estimated to be 5.7 kJ mol^{-1}. The potential barrier to internal rotation of the "free" CH_3 is determined to be 2.244 kcal mol^{-1} (or 784.9 cm^{-1}).



[a]) Uncertainties were not estimated in the original paper.
[b]) Distance between the two carbon atoms out of symmetry plane.
[c]) See figure for the definition.

Tatamitani, Y., Liu, B., Shimada, J., Ogata, T., Ottaviani, P., Maris, A., Caminati, W., Alonso, J.L.: J. Am. Chem. Soc. **124** (2002) 2739.