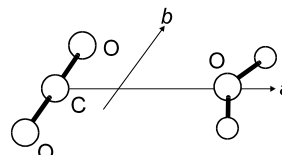


105
MW**CH₂O₃****Carbon dioxide – water (1/1)**
(weakly bound complex)**C_{2v}**
(effective symmetry class)
(large-amplitude motion)
CO₂ · H₂O

r_0	Å ^{a)}	θ_0	deg ^{a)}
C...O	2.838(5)	H–O–H	104.5 ^{b)}
O–H	0.9590(20)	O=C=O	180 ^{b)}
C=O	1.1614 ^{b)}		

Atom	a_0 [Å]	b_0 [Å]
H	2.5816	±0.7583
O (in CO ₂)	–0.8435	±1.1614



The MW spectrum of a T-shaped water-carbon dioxide complex has been recorded and analyzed. The rotational spectra show a splitting of the energy levels from internal rotation between the water and carbon dioxide molecules around the van der Waals bond of the complex. A barrier equivalent to 285.6(14) cm^{–1} has been adjusted with the help of a flexible model for the internal rotation in the complex of water about its C₂ symmetry axis. The van der Waals bond length has been allowed to vary during the least-squares fit of internal rotation parameters.

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Assumed.

Columberg, G., Bauder, A., Heineking, N., Stahl, W., Makarewicz, J.: Mol. Phys. **93** (1998) 215.

[II/25B\(3, 233\)](#)