

329	C₂O₂	Carbon monoxide dimer	C₂
MW		(weakly bound complex)	(effective symmetry class)
			(large-amplitude motion)
			(CO) ₂

State $r_0(R_{\text{cm}})$ Å ^{a)}

$K=0$ 4.26(1)

$K=1$ 4.17(1)

For the vibrationally excited state, $\nu_{\text{CO}} = 1$, see [0], where it was reported that $R_{\text{cm}} = 4.35$ and 4.10 Å in $K = 0$ and 1 , respectively.

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

Roth, D.A., Surin, L.A., Dumesh, B.S., Winnewisser, G., Pak, I.: J. Chem. Phys. **113** (2000) 3034.

[0] Walker, K.A., Xia, C., McKellar, A.R.W.: J. Chem. Phys. **113** (2000) 6618.

C_s
(effective symmetry class)

Nine rotational-tunneling states have been confirmed to exist in the ground state ($\nu_{\text{CO}} = 0$) manifold. The observation of dramatically different intensities for different bands supports the concept of two isomeric forms for (CO)₂, the ground state having a larger intermolecular separation (*ca.* 4.4 Å) with most likely a C-bonded configuration, and the low-lying (0.88 cm^{-1}) excited state having a smaller separation (*ca.* 4.0 Å) and an O-bonded geometry.

Tang, J., McKellar, A. R. W., Surin, L.A., Fourzikov, D.N., Dumesh, B.S., Winnewisser, G.: J. Mol. Spectrosc. **214** (2002) 87.

IR

(effective symmetry class)

Isotopic species	Isomer I		Isomer II		Reference
	Band origin [cm^{-1}]	R_{cm} [Å] ^{a)}	Band origin [cm^{-1}]	R_{cm} [Å] ^{a)}	
¹² C ¹⁶ O · ¹² C ¹⁶ O	0	4.34(5)	0.8770	4.09(5)	[1]
	2.5321	4.44(5)	2.7805	3.99(5)	
	2143.8944	4.43(5)	2142.8727	4.01(5)	
	2146.1539	4.51(5)	2145.1472	3.95(5)	
	2146.6313	4.25(5)			
	2152.9343	4.49(5)			
¹³ C ¹⁶ O · ¹² C ¹⁶ O	0	4.40(5)			[1]
	2144.0386	4.35(5)			
	2146.0619	4.54(5)			
¹³ C ¹⁶ O · ¹³ C ¹⁶ O	0	4.424(10)	1.2851	4.013(10)	[2]
	2.3575	4.475(10)	2096.0541	4.163(10)	
	2096.7307	4.252(10)	2098.2885	3.972(10)	
	2098.7026	4.475(10)			
	2099.5674	4.279(10)			
	2105.1009	4.453(10)			
¹² C ¹⁸ O · ¹² C ¹⁸ O	0	4.307(10)	0.6386	4.093(10)	[3]
	2092.6697	4.498(10)	2091.5792	3.948(10)	
	2094.8468	4.541(10)	2093.5388	3.910(10)	
	2096.5665	4.077(10)	2095.3456	4.216(10)	
			2097.3573	4.375(10)	

The structures were determined from the supersonic spectra in the region of the CO stretching vibration. The geometries of the monomer subunits were assumed to be unchanged upon complexation. Using the temperature dependence and the method of combination differences, rotational levels for the ground state ($\nu_{\text{CO}}=0$) and the excited vibrational state ($\nu_{\text{CO}}=1$) were assigned. The levels form two groups, corresponding to isomers with effective intermolecular separations of either *ca.* 4.4 or 4.0 Å. The first isomer is the ground state, whereas the isomer with $R_{\text{cm}} = 4.0$ Å is a low-lying excited state. Previous calculations suggest that both forms are planar and roughly T-shaped. The ground state forms a C-bonded configuration, whereas the excited state exhibits an O-bonded configuration.

^a) Uncertainties were not given in the original papers.

[1] Brookes, M.D., McKellar, A.R.W.: J. Chem. Phys. **111** (1999) 7321.

[2] McKellar, A.R.W.: J. Chem. Phys. **115** (2001) 3571.

[3] McKellar, A.R.W.: J. Mol. Spectrosc. **226** (2004) 190.

Replaces [II/25B\(3, 986\)](#)