

20  
MWCClFO<sub>2</sub>

Carbon dioxide – chlorine fluoride (1/1)

(weakly bound complex)

(effective symmetry class)  
(large-amplitude motion)C<sub>∞v</sub>  
CO<sub>2</sub> · ClF

Isotopic species	$r_0(R_{\text{cm}})$ [Å]	$r_0(\text{O} \cdots \text{Cl})$ [Å]	$\theta_0(\varphi)$ [deg] <sup>a) b)</sup>
<sup>12</sup> CO <sub>2</sub> · <sup>35</sup> ClF	4.436(2)	2.699(2)	11.7(5) <sup>c)</sup>
<sup>12</sup> CO <sub>2</sub> · <sup>37</sup> ClF	4.415(2)	2.698(2)	
<sup>13</sup> CO <sub>2</sub> · <sup>35</sup> ClF	4.437(2)	2.699(2)	

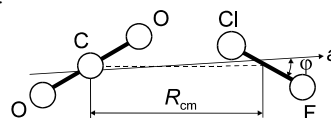
The complex is a linear or nearly linear molecule. Interpretation of the spectroscopic constants reveals that the nuclei lie in the order OCO · ClF and that the intermolecular bond is very easily distorted both radially and angularly.

The intermolecular stretching force constant is 0.775 N m<sup>-1</sup>.

<sup>a)</sup> Uncertainty was not estimated in the original paper.

<sup>b)</sup> See figure for the definition.

<sup>c)</sup> Average value.



Cooke, S.A., Legon, A.C., Holloway, J.H.: J. Mol. Struct. **406** (1997) 15.