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IR

 C_3O_6

 Carbon dioxide trimer
(weakly bound complex)

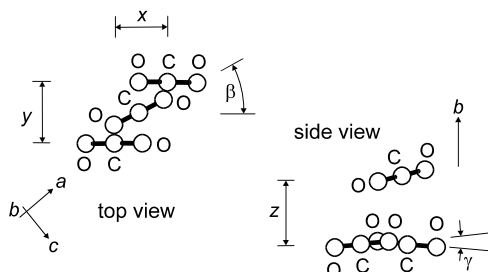
 C_2
(effective symmetry class)
(large-amplitude motion)
 $3(\text{CO}_2)$

r_0	\AA^{a}	θ_0	deg^{a}
x^{b}	2.380(43)	β^{b}	27.1(69)
y^{b}	2.913(43)	γ^{b}	5.8(40)
z^{b}	3.017(28)		

The non-cyclic structure was determined from two rovibrational bands corresponding to the two most IR-active linear combinations of the three constituent CO_2 monomer asymmetric stretches. The C_2 symmetry axis was established due to the nuclear spin statistics of the rovibrational transitions. The geometries of the monomer subunits were assumed to be unchanged upon complexation.

^a) Estimated standard errors.

^b) See figure for the definition.



Weida, M.J., Nesbitt, D.J.: J. Chem. Phys. **105** (1996) 10210.

[II/25C \(3, 1457\)](#)