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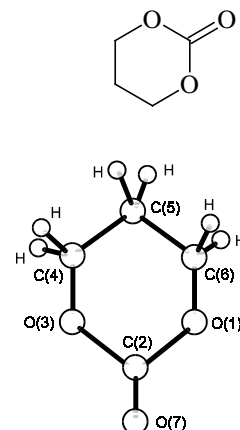
C₄H₆O₃

1,3-Dioxan-2-one
Trimethylene carbonate

C_s

r_a	Å ^{a)}	θ_a	deg ^{a)}
C(2)=O(7)	1.19(2)	O(1)–C(2)=O(7)	127(2)
C(2)–O(1)	1.395(8)	C(2)–O(3)–C(4)	122(3)
C(4)–O(3)	1.45(2)	C(4)–C(5)–C(6)	109(4)
C(4)–C(5)	1.53(2)	O(3)–C(4)–C(5)	112(3)
C–H	1.13 ^{b)}	O(1)–C(2)–O(3)	106 ^{c)}
		α ^{d)}	130 ^{c)}
		β ^{e)}	140 ^{c)}

The experimental data agree with the chair and envelope conformations and show a somewhat better agreement with the former model, but no full agreement with the data based on the dipole moment and the Kerr effect has been achieved. The data based on the model of the chair conformation are listed. The temperature of the measurement was not stated.



^{a)} The uncertainties are unidentified, possibly estimated standard errors, and are larger than those listed in the original data.

^{b)} Assumed.

^{c)} Dependent parameter.

^{d)} Dihedral angle between the planes C(6)O(1)O(3)C(4) and O(1)C(2)O(3).

^{e)} Dihedral angle between the planes C(4)C(5)C(6) and C(6)O(1)O(3)C(4).

Arbuzov, B.A., Anonimova, I.V., Tuzova, L.L., Naumov, V.A., Yarkova, E.G., Safiullina, N.R., Timosheva, A.P., Vereshchagin, A.N.: *Izv. Akad. Nauk SSSR, Ser. Khim.* (1984) 2705; *Proc. Acad. Sci. USSR, Chem. Ser. (Engl. Transl.)* (1984) 2476.