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# Cyclopentene-1,2,3-trione, $C_5H_2O_3$

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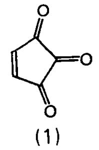
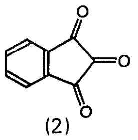
**Abstract.** $M_r = 110\cdot07$, tetragonal $P4_12_12$, $a = b = 5\cdot701\,(1)$, $c = 14\cdot113\,(2)$ Å, $V = 458\cdot7\,(2)$ Å$^3$, $Z = 4$, $D_x = 1\cdot59$ Mg m$^{-3}$, Mo $K\alpha$, $\lambda = 0\cdot71073$ Å, $\mu = 0\cdot127$ mm$^{-1}$, $F(000) = 224$, $T = 295$ K, $R = 0\cdot037$ for 253 observed reflections $[I > 2\cdot5\sigma(I)]$. The crystal structure was solved by trial and error because direct methods failed. Cyclopentene-1,2,3-trione has twofold symmetry in the crystal. The cyclopentene group is planar with normal bond lengths and angles. The carbonyl groups are also in this plane. Close interactions exist between carbonyl groups of neighbouring molecules producing a helical arrangement parallel to **c**.

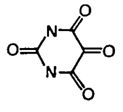
**Introduction.** The O···O distances of the carbonyl groups in cyclopentene-1,2,3-trione (1) are important to the electronic interactions within the molecule (Gleiter, Dobler & Eckert-Maksić, 1982). There is an additional interest in (1) regarding the crystal structure because strong O···C=O interactions between neighbouring molecules in the crystal have been found for 1,2,3-indantrione (2) (Bolton, 1965), alloxan (3) (Bolton, 1964) and 4,6-cycloheptadiene-1,2,3-trione (4) (Hirama, Fukazawa & Itô, 1978).



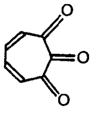
(1)



(2)



(3)



(4)

**Experimental.** Red crystal 0·35 × 0·35 × 0·30 mm, grown by sublimation in vacuum; CAD-4 diffractometer (Enraf–Nonius), cell dimensions from $2\theta$ angles of 25 reflections $(16 < 2\theta < 38°)$; 1649 data up to $2\theta = 64°$ (excluding systematic absences), $0 \le h \le 4$, $0 \le k \le 8$, $0 \le l \le 18$, 3 standard reflections 004, $\bar{1}14$, 220 (max. variation 0·99 to 1·036), 501 unique reflections $(R_{\text{int}} = 0\cdot027)$, no absorption correction, 253 intensities with $I > 2\cdot5\sigma(I)$. Structure solution by direct methods (*MULTAN*80; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) failed, probably because the contents of the cell differ too greatly from random distribution owing to high crystallographic symmetry and planar arrangement of the atoms within the molecule. Models were built complying with the following requirements: (1) there are four molecules in the unit cell, hence they have to lie on twofold axes; (2) the inclination of the planar molecule is known fairly well, because the four reflections 114, 228, 3,3,11 and 4,4,15 are among the five with the highest $E(hkl)$ values. One of the possible models was the solution of the structure. It was refined by full-matrix least squares on $F^2$ with anisotropic thermal parameters for C and O atoms. H atom located by difference Fourier syntheses and refined isotropically. 40 parameters, $R = 0\cdot037$ for 253 observed reflections, $wR = 0\cdot064$, $w = 4F^2/\sigma^2(F^2) + (0\cdot03F^2)^2$, $S = 2\cdot44$, $\Delta/\sigma < 0\cdot01$, largest peak = 0·16 e Å$^{-3}$;* scattering factors from *International Tables for X-ray Crystallography* (1974); *SDP* programs (Frenz, 1978) used on PDP11/44.

**Discussion.** Final atomic parameters are given in Table 1. Bond lengths, bond angles and the numbering system of cyclopentene-1,2,3-trione (1) are depicted in Fig. 1. Owing to space-group symmetry, the molecule lies on a twofold axis. The five-membered ring is planar within ±0·009 (4) Å. This is in good agreement with 1,2,3-indantrione (2) (Bolton, 1965). The O···O distances of adjacent carbonyl groups in five- and six-membered cyclic 1,2,3-triones [(1) 2·942 (4); (2) 2·941 (9) (Bolton, 1965); (3) 2·747 (7) Å (Bolton, 1964)] are not essentially shorter than the van der Waals distance [2·8 Å (Pauling, 1976)]. In all these compounds a planar arrangement of the carbonyl groups is possible. On the other hand, a twist of the seven-membered ring has been found in (4) (O···O 2·605 and 2·637 Å) (Hirama, Fukazawa & Itô, 1978).

The central C=O bond is shorter than the terminal ones in the compounds (2) to (4). The structure of (1) also shows this difference, but it is not significant.

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* Lists of structure factors and anisotropic thermal parameters and a packing diagram have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39446 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Atomic coordinates and thermal parameters*

$U_{eq}$ is one third of the trace of the orthogonalized $U_{ij}$ tensor.

|  | $x$ | $y$ | $z$ | $U_{eq}$(Å$^2$ × 10$^3$) |
|---|---|---|---|---|
| O(1) | 0·4697 (5) | 0·4697 (5) | 0·0000 | 49 (1) |
| O(2) | 0·0269 (5) | 0·4768 (5) | 0·1070 (2) | 46 (2) |
| C(1) | 0·3210 (7) | 0·3210 (7) | 0·0000 | 32 (1) |
| C(2) | 0·0915 (7) | 0·3212 (7) | 0·0550 (2) | 31 (2) |
| C(3) | −0·0246 (6) | 0·1004 (7) | 0·0310 (3) | 36 (2) |
|  |  |  |  | $U_{iso}$(Å$^2$ × 10$^2$) |
| H(3) | −0·182 (6) | 0·049 (8) | 0·056 (3) | 7 (1) |

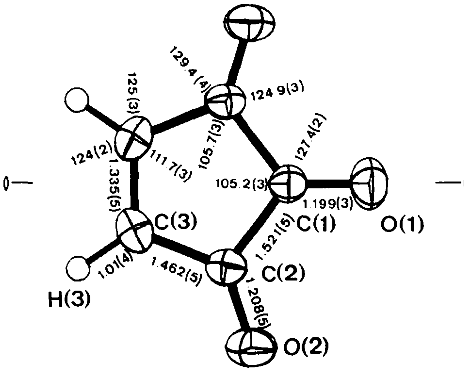

Fig. 1. *ORTEP* plot (Johnson, 1970) of (1) with 50% probability thermal ellipsoids showing bond lengths (Å), bond angles (°) and the numbering system.

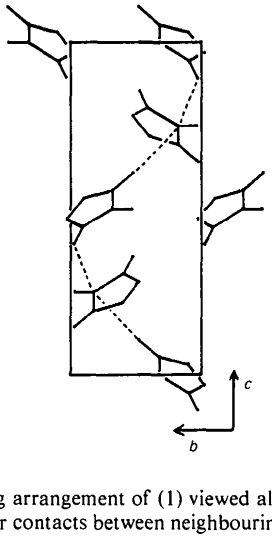

Fig. 2. The packing arrangement of (1) viewed along **a** showing the intermolecular contacts between neighbouring molecules.

There are close intermolecular O···C=O interactions in the crystal structure of (1) like those found in cyclic 1,2,3-triones [(2) 2·85 (1) (Bolton, 1965); (3) 2·79–3·01 $(0_7)$ (Bolton, 1964); (4) 2·77–2·96 Å (Hirama, Fukazawa & Itô, 1978)]. In the structure of (1) each molecule has four close links to its four nearest neighbours. These interactions are crystallographically equivalent with a distance of 2·946 (4) Å [van der Waals distance 3·1 Å (Pauling, 1976)] and with an O···C=O angle of 105·2 (1)°. The intermolecular contacts are between the C(1) atom of the central carbonyl group and the oxygen atoms $O(2^{i})$ and $O(2^{ii})$ of the terminal carbonyl groups of molecules lying above and below the molecular plane of (1) [(i) $-0{\cdot}5+y$, $0{\cdot}5-x$, $-0{\cdot}25+z$; (ii) $0{\cdot}5-x$, $-0{\cdot}5+y$, $0{\cdot}25-z$)]. These links produce the helical arrangements along the twofold screw axes parallel to **c** (Fig. 2). Owing to space-group symmetry the contacts are equal; hence there is no deformation of the planar arrangement of the central carbonyl group in contrast to compounds with a one-sided interaction (Bürgi, Dunitz & Shefter, 1974).

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