All the computations were carried out on an IBM 1620 computer with a unified set of crystallographic programs developed by Ahmed, Gabe, Mair & Pippy (1963). The authors are indebted to Dr R. A. Shaw of Birkbeck College, London for stimulating their interest in the problem and for supplying the specimens. Grateful acknowledgement is made to Mrs M. E. Pippy for assistance with the computations, and to the staff of the N. R. C. Computation Centre for their cooperation.

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The Crystal Structure of Succinic Anhydride

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The crystal structure of succinic anhydride, $(CH_2CO)_2O$, which is isomorphous with maleic anhydride, has been determined and refined with the use of three-dimensional X-ray data. The crystals are orthorhombic with cell dimensions $a = 6\cdot963$, $b = 11\cdot710$, $c = 5\cdot402$ Å. The space group is $P2_12_12_1$. The molecular arrangement is similar to that of maleic anhydride.

The thermal vibrations of the molecule are discussed.

Introduction

The structure of maleic anhydride has recently been published by Marsh, Ubell & Wilcox (1962). Lonsdale, (1939), referring to unpublished work by Monvoisin, states that maleic and succinic anhydride are isomorphous although the latter substance has two more hydrogen atoms in the molecule and the corresponding acids have different configurations. It appeared therefore of particular interest to compare the structures of succinic anhydride and maleic anhydride, and a detailed structure determination of succinic anhydride was undertaken.

Experimental

Crystal data

Succinic anhydride $(CH_2CO)_2O$
M.W. 100·08
Orthorhombic
$a = 6\cdot963 \pm 0\cdot015$ Å
$b = 11\cdot71 \pm 0\cdot04$
$c = 5\cdot402 \pm 0\cdot010$

(The errors given are three times the standard errors of averages).

Density (calculated, $Z = 4$) $1\cdot509$ g.cm^{-3}
Density (measures) $1\cdot505$ g.cm^{-3} (S.T.P.)

Total number of electrons per unit cell $= F(000) = 208$

Systematic absences:
$h00$: $h = 2n + 1$
$0k0$: $k = 2n + 1$
$00l$: $l = 2n + 1$
Space group: $P2_12_12_1$
Molecular symmetry: none.

Description of crystals

Crystals were grown from a hot solution of commercial succinic anhydride and chloroform. Most crystals were needle-shaped, but for the X-ray work two almost equidimensional crystals of $0\cdot4 \times 0\cdot4 \times 0\cdot45$ mm^3 and $0\cdot54 \times 0\cdot61 \times 0\cdot67$ mm^3 respectively were found. They were somewhat hygroscopic, and were therefore coated with collodion, which proved sufficient protection against the moisture in the atmosphere during the time needed for the experimental work.

The density was determined by Yardley (1924) by flotation of crystals in a mixture of benzene and methylene iodide. The result given for the specific gravity ϱ is

$$1{\cdot}508 > \varrho < 1{\cdot}501\ .$$

X-ray data

The unit-cell dimensions were determined from rotation photographs and high order reflexions on Weissenberg photographs.

From one crystal, mounted about the *c* axis, Weissenberg photographs were taken for $l=0$–3 and from a second crystal, mounted about the *b* axis, photographs for $k=0$–8. In both cases the respective zero layers were retaken and the results confirmed that the coating had been sufficient to prevent any substantial change in the crystal.

Film packs were used and 220 and 348 reflexions with observable intensities were recorded from the two sets of photographs, giving 390 independent reflexions. This is 65% of all possible reflexions in the Cu $K\alpha$ sphere. The intensities of the reflexions were estimated by visual comparison with an intensity scale. These values were corrected by the appropriate Lorentz–polarization factors and the Phillips correction, which applies to the peak blackening of the spots and makes allowance for their extension on upper-layer Weissenberg photographs. (Phillips, 1954, 1956). It was found that when the Phillips correction was applied with Phillips's value for the parameter $\mathscr{R}_2$, spots with low *h* and *l* indices recorded on layers with large *k* values were systematically over-corrected, as compared with the same spots recorded ou the *c* axis Weissenberg photographs. It appears therefore that visual estimation does not strictly give an estimate of the maximum blackening, but a value between this and the integrated intensity. In consequence the parameter $\mathscr{R}_2$ was reduced so as to minimize the systematic differences. The validity of Phillips's value for this parameter was also questioned by Lonsdale (1964).

Structure analysis

Comparison between maleic anhydride and succinic anhydride showed marked similarity, not only in the cell dimensions, but also in the distribution of intensities. A molecular arrangement similar to that of maleic anhydride was therefore used as a trial structure for succinic anhydride. Initial calculations, using reflexions falling within increasing ranges of $\sin\theta/\lambda$ and isotropic *B* factors gave a discrepancy index of 13%. Four cycles of refinement using anisotropic temperature factors for carbon and oxygen atoms and including the contribution of hydrogen atoms with isotropic temperature factors, improved the *R* index to 7·6%. Neither the hydrogen positions nor their temperature factors were refined. Unit weights were used throughout, and no correction was made for extinction, but 20 low angle reflexions of high intensities were left out of the refinement. It is assumed that a correction for extinction would not alter the atomic coordinates, nor the relative temperature factors. Calculation of structure factors for the unobserved reflexions showed that their values are below the lowest observable value. The final parameters and their standard deviations are given in Table 1, and the observed and calculated structure factors in Table 2.

Table 1. *Final parameters and standard deviations, as comptend*

(*a*) Fractional coordinates

	x/a	σ_x	y/b	σ_y	z/c	σ_z
C(1)	0·1655	0·0010	0·2119	0·0006	0·3422	0·0012
C(2)	0·0300	0·0010	0·1786	0·0006	0·1475	0·0012
C(3)	−0·0391	0·0009	0·0608	0·0006	0·2196	0·0012
C(4)	0·0603	0·0010	0·0373	0·0006	0·4572	0·0012
O(5)	0·1768	0·0006	0·1272	0·0004	0·5204	0·0008
O(6)	0·2596	0·0008	0·2963	0·0004	0·3643	0·0011
O(7)	0·0527	0·0009	−0·0436	0·0005	0·5900	0·0010
H(8)	0·0982		0·1801		−0·0258	
H(9)	−0·0747		0·2380		0·1241	
H(10)	−0·0155		0·0021		0·0808	
H(11)	−0·1883		0·0601		0·2307	

(*b*) Components of vibration ellipsoid tensor

$$T=\exp\,\{-(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{23}kl+b_{31}hl+b_{12}hk)\}$$

	b_{11}	b_{22}	b_{33}	b_{23}	b_{31}	b_{12}
C(1)	0·0176	0·0080	0·0324	−0·0041	0·0020	0·0008
C(2)	0·0206	0·0085	0·0247	−0·0006	−0·0086	−0·0011
C(3)	0·0175	0·0093	0·0262	−0·0038	−0·0060	−0·0001
C(4)	0·0205	0·0076	0·0326	0·0037	0·0076	0·0061
O(5)	0·0170	0·0092	0·0269	−0·0027	−0·0033	0·0011
O(6)	0·0289	0·0100	0·0531	−0·0067	−0·0075	−0·0074
O(7)	0·0308	0·0112	0·0503	0·0104	0·0014	0·0038

Discussion

Bond distances and bond angles

Bond distances and angles are shown in Fig. 1. The standard deviations of the bond lengths are 0·01 Å in every case. The C–O and C=O bonds, as well as the bonds C(1)–C(2) and C(3)–C(4) agree with those found in maleic anhydride and other related compounds. The single bond between C(2) and C(3) also has a normal value of 1·51 Å. A list of deviations from the mean plane through all seven atoms is given in Table 3. A deviation from planarity is indicated by values of −0·014 Å for C(2) and +0·013 Å for C(3), while in maleic anhydride this part of the molecule is planar.

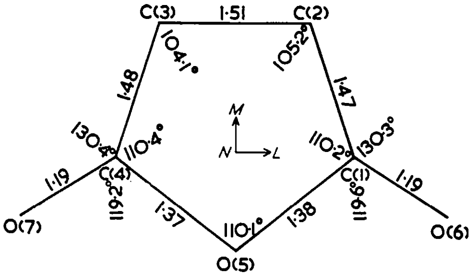

Fig. 1. Bond distances (Å) and angles (°) and molecular axes *L*,*M*,*N* through the centre of inertia.

Table 2. *Observed and calculated structure factors*

The values listed are half the absolute values. All reflexions in the Cu sphere not listed have observed and calculated values below the lowest recorded value; those marked with an asterisk were omitted from the least-square refinements.

H	K	L	F OBS	F CALC	COS α	SIN α
0	0	0	——	104.00		
2	0	0	7.84	8.20	1.00	0.00
4	0	0	7.95	7.72	1.00	0.00
6	0	0	2.43	1.93	1.00	0.00
8	0	0	2.62	2.74	-1.00	0.00
1	0	1	*12.51	16.20	0.00	1.00
2	0	1	*16.01	20.32	0.00	-1.00
3	0	1	3.73	3.44	0.00	1.00
4	0	1	0.73	0.47	0.00	1.00
5	0	1	2.52	2.19	0.00	1.00
6	0	1	2.75	2.69	0.00	-1.00
7	0	1	0.90	1.07	0.00	1.00
8	0	1	1.23	1.28	0.00	-1.00
0	0	2	7.55	8.30	1.00	0.00
1	0	2	8.82	10.01	1.00	0.00
2	0	2	2.29	2.29	-1.00	0.00
3	0	2	7.52	7.93	-1.00	0.00
4	0	2	3.00	2.85	-1.00	0.00
8	0	2	1.32	1.38	-1.00	0.00
1	0	3	4.63	4.85	0.00	-1.00
2	0	3	2.85	2.98	0.00	-1.00
5	0	3	0.94	1.01	0.00	-1.00
6	0	3	1.79	1.90	0.00	-1.00
0	0	4	1.54	1.78	-1.00	0.00
1	0	4	4.00	4.14	-1.00	0.00
4	0	4	2.36	1.99	-1.00	0.00
5	0	4	1.41	1.30	1.00	0.00
7	0	4	1.10	1.02	-1.00	0.00
1	0	5	1.32	1.21	0.00	-1.00
2	0	5	2.35	2.02	0.00	-1.00
3	0	5	1.71	1.89	0.00	1.00
4	0	5	1.61	0.96	0.00	1.00
5	0	5	1.48	1.46	0.00	-1.00
6	0	5	1.25	0.82	0.00	-1.00
0	0	6	2.29	2.00	1.00	0.00
1	0	6	1.11	0.91	-1.00	0.00
2	0	6	1.48	1.33	-1.00	0.00
3	0	6	2.57	2.44	1.00	0.00
1	1	0	*12.14	12.62	0.00	1.00
2	1	0	*12.08	12.70	-1.00	0.00
3	1	0	10.63	10.51	0.00	1.00
4	1	0	5.98	5.78	1.00	0.00
7	1	0	2.30	2.35	0.00	1.00
8	1	0	1.56	1.93	-1.00	0.00
0	1	1	*11.85	14.08	0.00	-1.00
1	1	1	*18.16	21.68	-0.75	-0.66
2	1	1	*18.33	18.78	0.24	0.07
3	1	1	5.24	5.06	0.69	0.72
4	1	1	3.29	3.49	0.98	0.19
5	1	1	1.17	1.57	-0.48	-0.88
6	1	1	2.01	2.12	0.77	-0.63
7	1	1	1.21	1.56	0.93	-0.36
0	1	2	*12.46	13.86	0.00	1.00
1	1	2	11.35	11.21	-0.24	0.97
2	1	2	7.46	6.41	-0.69	0.72
3	1	2	7.89	6.84	-0.56	0.83
4	1	2	3.89	3.73	0.50	0.87
5	1	2	2.89	3.14	-0.43	0.90
6	1	2	1.27	1.15	-1.00	0.05
7	1	2	1.99	2.55	0.16	0.99
0	1	3	1.36	1.57	0.00	-1.00
1	1	3	7.84	7.10	-0.91	-0.42
2	1	3	6.29	6.43	0.07	-1.00
4	1	3	1.74	1.85	-0.96	-0.27
5	1	3	3.12	3.19	-0.46	-0.89
6	1	3	1.71	1.50	-0.73	-0.68
1	1	4	2.37	2.35	0.70	0.71
2	1	4	2.59	2.45	-0.12	-0.99
3	1	4	4.51	4.60	0.85	-0.53
4	1	4	2.20	2.25	0.77	-0.64
5	1	4	1.21	1.74	-0.05	-1.00
0	1	5	1.27	1.25	0.00	-1.00
1	1	5	3.70	3.81	0.39	0.92
2	1	5	1.26	1.35	0.92	0.40
3	1	5	2.11	2.43	0.99	-0.12
4	1	5	1.12	1.20	-0.58	0.82
2	1	6	1.73	1.77	-0.96	-0.29
3	1	6	1.08	1.07	1.00	0.04
0	2	0	1.35	0.96	1.00	0.00
1	2	0	*16.53	20.73	0.00	1.00
2	2	0	*20.04	23.90	1.00	0.00
3	2	0	7.09	7.03	0.00	-1.00
5	2	0	5.04	5.20	0.00	1.00
6	2	0	1.65	2.01	-1.00	0.00
8	2	0	1.26	1.42	-1.00	0.00
0	2	1	*12.49	13.25	-1.00	0.00
1	2	1	8.16	8.27	0.88	-0.47
2	2	1	*15.28	14.96	-0.88	-0.47
3	2	1	1.98	2.05	-0.40	0.92
4	2	1	8.18	8.02	-0.11	-0.99
5	2	1	4.75	5.01	-1.00	-0.01
6	2	1	3.33	3.49	-0.40	-0.92
7	2	1	2.06	2.21	0.88	-0.47
0	2	2	6.36	6.63	1.00	0.00
1	2	2	11.01	11.20	-0.99	-0.10
2	2	2	2.63	2.80	0.54	0.84
3	2	2	8.88	8.47	0.43	-0.90
4	2	2	1.04	1.09	-0.35	0.94
5	2	2	1.14	0.93	0.48	0.87
1	2	3	7.43	7.96	0.80	-0.60
2	2	3	4.36	4.22	-0.89	-0.45
3	2	3	2.36	2.15	-0.56	-0.83
4	2	3	1.14	1.33	0.17	0.99
6	2	3	1.11	1.35	0.52	0.86
0	2	4	5.31	5.71	1.00	0.00
1	2	4	2.07	2.33	0.60	0.80
2	2	4	1.14	1.29	-0.50	-0.87
3	2	4	2.02	2.02	-0.40	-0.92
4	2	4	2.61	2.83	0.48	0.88
0	2	5	1.18	1.27	1.00	0.00
1	2	5	4.04	4.31	0.61	0.79
0	2	6	2.39	2.67	-1.00	0.00
1	2	6	1.51	1.79	0.62	0.79
3	2	6	0.96	0.84	0.57	-0.82
4	2	6	2.01	1.95	-0.19	0.98
1	3	0	1.98	2.12	0.00	-1.00
2	3	0	2.39	2.19	1.00	0.00
4	3	0	5.96	5.74	1.00	0.00
5	3	0	6.54	6.11	0.00	1.00
6	3	0	1.06	1.12	1.00	0.00
7	3	0	3.46	3.50	0.00	-1.00
8	3	0	1.54	1.61	1.00	0.00
0	3	1	2.75	1.78	0.00	1.00
1	3	1	*13.37	13.42	-0.65	0.76
2	3	1	7.41	6.47	1.00	0.06
3	3	1	*13.43	11.63	-0.97	-0.25
4	3	1	3.98	3.47	0.53	0.85
5	3	1	2.80	2.94	0.99	0.15
6	3	1	2.31	2.37	0.91	-0.42
7	3	1	1.69	1.91	0.64	0.77
8	3	1	1.46	1.48	0.80	0.59
0	3	2	5.54	5.10	0.00	-1.00
1	3	2	5.16	4.56	0.80	-0.60
2	3	2	8.30	7.59	-0.94	0.35
3	3	2	7.77	6.80	0.66	0.75
4	3	2	4.56	4.18	0.24	-0.97
5	3	2	3.66	3.51	-0.27	0.96
6	3	2	2.33	2.12	-0.88	0.47
7	3	2	1.29	1.35	-0.97	0.26
8	3	2	1.31	1.23	-0.96	-0.31
0	3	3	11.13	11.28	0.00	-1.00
1	3	3	2.00	1.98	0.91	0.42
2	3	3	3.53	3.09	-0.11	0.99
3	3	3	5.78	5.34	0.12	-0.99
5	3	3	3.64	3.19	0.48	-0.88
6	3	3	0.97	1.15	-0.12	-0.99
7	3	3	0.94	0.98	0.39	-0.92
0	3	4	1.00	1.16	0.00	-1.00
1	3	4	5.09	4.67	0.78	-0.62
2	3	4	2.65	2.62	-0.91	0.41
3	3	4	2.88	2.57	0.70	0.72
4	3	4	2.08	1.93	0.72	0.70
0	3	5	1.05	1.03	0.00	-1.00
1	3	5	2.33	2.02	0.90	-0.44
2	3	5	3.02	2.76	-0.89	0.46
5	3	5	0.88	0.79	0.90	-0.43
6	3	5	0.80	0.93	-0.99	0.15
1	3	6	1.31	1.43	-0.61	-0.79
4	3	6	0.95	0.95	-0.40	0.92
0	4	0	7.07	6.91	1.00	0.00
1	4	0	7.63	7.00	0.00	-1.00
2	4	0	5.96	5.51	1.00	0.00
3	4	0	2.20	2.25	0.00	1.00
4	4	0	2.30	2.17	1.00	0.00
5	4	0	2.19	2.27	0.00	-1.00
6	4	0	2.55	2.64	-1.00	0.00
7	4	0	0.85	1.02	0.00	-1.00
0	4	1	*9.81	9.61	-1.00	0.00
1	4	1	3.55	3.50	0.99	0.13
2	4	1	1.36	1.12	-0.17	0.99
3	4	1	3.07	3.11	-0.54	-0.84
4	4	1	8.96	8.21	-0.47	-0.88
5	4	1	3.79	3.38	1.00	0.08
6	4	1	2.61	2.78	1.00	-0.09
0	4	2	5.27	4.97	-1.00	0.00
1	4	2	6.75	6.37	0.94	-0.34
2	4	2	7.48	6.64	0.94	0.35
3	4	2	2.77	2.68	-0.64	-0.77
4	4	2	8.41	7.21	0.23	0.97
5	4	2	0.93	0.62	-0.78	-0.62
6	4	2	3.30	3.60	-0.69	0.72
7	4	2	0.94	0.86	1.00	0.05
8	4	2	0.90	0.90	0.63	0.78
0	4	3	2.87	2.74	-1.00	0.00
1	4	3	1.09	1.35	-0.90	0.45
2	4	3	4.48	4.17	0.16	0.99
3	4	3	2.04	2.19	0.79	-0.61
4	4	3	3.36	3.24	-0.10	-1.00
5	4	3	2.88	2.94	-0.99	0.16
6	4	3	1.17	1.38	0.97	-0.25
0	4	4	4.91	4.56	-1.00	0.00
1	4	4	5.84	5.64	0.13	0.99
2	4	4	3.52	3.22	0.83	0.55
3	4	4	1.46	1.66	0.10	1.00
4	4	4	0.90	0.47	0.76	-0.64
5	4	4	1.16	0.84	0.21	0.97
6	4	4	1.13	1.06	-0.99	-0.16
0	4	5	4.29	4.18	-1.00	0.00
1	4	5	1.57	1.47	-0.02	1.00
2	4	5	3.34	3.49	-0.94	0.34
3	4	5	1.44	1.56	0.99	0.11
4	4	5	0.73	0.62	-0.37	-0.92
5	4	5	1.16	1.03	0.91	0.41
0	4	6	0.86	1.06	-1.00	0.00
1	4	6	1.09	1.34	0.49	-0.87
2	4	6	0.63	0.74	-0.27	0.97
3	4	6	0.54	0.41	1.00	0.04
1	5	0	5.97	5.73	0.00	-1.00
2	5	0	*9.14	8.08	1.00	0.00
3	5	0	*10.04	9.59	0.00	1.00
4	5	0	0.89	1.08	1.00	0.00
6	5	0	3.15	3.31	1.00	0.00
7	5	0	2.03	2.10	0.00	1.00
8	5	0	0.95	1.25	1.00	0.00
0	5	1	4.60	4.94	0.00	1.00
1	5	1	1.98	2.11	0.48	-0.88
2	5	1	5.32	5.10	-0.96	-0.29
3	5	1	1.21	1.10	-0.79	0.61
4	5	1	1.18	1.24	0.94	-0.34
5	5	1	1.92	1.97	0.56	0.83
6	5	1	2.03	2.20	-0.70	0.71
8	5	1	0.89	1.19	-0.97	-0.22
0	5	2	3.91	3.84	0.00	1.00
1	5	2	8.29	8.11	0.89	-0.46
2	5	2	1.25	1.26	0.98	-0.20
3	5	2	1.81	1.55	1.00	0.05
4	5	2	7.08	6.51	-0.75	0.67
5	5	2	1.66	1.57	0.16	0.99
6	5	2	2.33	2.40	-.46	-0.89
7	5	2	1.12	1.41	-0.15	-0.99
8	5	2	0.70	0.85	-0.19	0.98
0	5	3	2.25	2.23	0.00	1.00
1	5	3	3.82	3.79	0.31	-0.95
2	5	3	3.28	3.40	-0.35	-0.94
3	5	3	6.36	6.06	-0.85	-0.54
4	5	3	0.83	0.90	0.90	-0.44
5	5	3	2.32	2.63	0.46	-0.89
6	5	3	1.82	2.00	-0.19	0.98
7	5	3	1.09	1.24	0.14	-0.99
0	5	4	1.15	1.17	0.00	-1.00
1	5	4	3.18	3.44	0.97	-0.25
3	5	4	1.75	1.72	0.56	-0.83
4	5	4	2.10	2.27	-0.93	-0.37
5	5	4	1.31	1.31	-0.02	1.00
0	5	5	0.80	0.99	0.00	1.00
1	5	5	0.79	0.75	-0.09	-1.00
2	5	5	0.77	0.75	0.47	-0.88
3	5	5	1.01	1.16	-0.62	-0.78
4	5	5	0.62	0.52	-0.61	0.80
5	5	5	0.56	0.64	0.40	-0.91
0	5	6	1.95	2.09	0.00	-1.00
2	5	6	0.63	0.50	-0.25	-0.97
3	5	6	1.11	1.09	-0.96	0.27
0	6	0	2.80	2.44	1.00	0.00
1	6	0	3.37	2.90	0.00	1.00
3	6	0	2.46	2.31	0.00	1.00
4	6	0	1.38	1.38	1.00	0.00
0	6	1	7.64	8.39	-1.00	0.00
1	6	1	7.30	7.40	-1.00	0.04
2	6	1	7.73	7.28	-0.99	0.12
3	6	1	3.11	2.99	0.96	0.29
4	6	1	2.16	1.85	0.64	0.77
6	6	1	1.69	2.01	-0.98	0.18
8	6	1	1.02	1.13	0.94	0.32
0	6	2	1.45	1.72	1.00	0.00
1	6	2	4.54	4.25	-0.08	-1.00
2	6	2	6.67	6.34	0.11	0.99
3	6	2	4.17	3.73	-0.48	0.88
5	6	2	3.03	2.95	-0.27	-0.96
6	6	2	1.14	1.38	0.15	0.99
7	6	2	1.25	1.13	-0.82	-0.57
0	6	3	3.30	3.37	-1.00	0.00
1	6	3	3.59	3.39	-0.60	0.80
2	6	3	2.87	2.76	-0.91	-0.41
3	6	3	1.22	1.34	0.18	0.98
4	6	3	1.38	1.46	0.78	-0.63
5	6	3	3.53	3.64	0.98	0.19
6	6	3	1.11	1.19	-0.30	-0.95
7	6	3	1.36	1.57	-1.00	-0.11
0	6	4	2.30	2.21	-1.00	0.00
2	6	4	2.21	2.09	-0.85	0.53
3	6	4	3.79	3.55	0.36	0.93
4	6	4	1.80	1.67	-0.58	0.82
5	6	4	1.70	1.79	0.45	-0.90
0	6	5	2.03	2.01	-1.00	0.00
3	6	5	1.23	1.35	0.80	-0.60
5	6	5	1.28	1.35	0.97	-0.25
0	6	6	0.95	0.87	1.00	0.00
2	6	6	0.98	1.19	0.44	0.89
1	7	0	5.05	5.28	0.00	1.00
2	7	0	1.13	1.28	1.00	0.00
3	7	0	2.67	3.01	0.00	-1.00
4	7	0	1.89	2.28	-1.00	0.00
5	7	0	2.16	2.33	0.00	1.00
0	7	1	4.09	4.13	0.00	1.00
1	7	1	3.61	3.22	0.17	-0.99
2	7	1	1.88	1.77	0.69	0.73
3	7	1	1.74	1.63	0.75	-0.66
4	7	1	3.49	3.52	-1.00	-0.00
5	7	1	1.90	1.80	-0.42	-0.91
6	7	1	1.58	1.88	-0.45	0.89
0	7	2	1.50	1.75	0.00	-1.00
1	7	2	3.11	2.84	0.66	0.75
3	7	2	2.56	2.34	-0.51	-0.86
4	7	2	4.02	3.78	-0.63	-0.77
5	7	2	2.50	2.80	-0.25	-0.97
6	7	2	1.65	1.65	-0.23	0.97
7	7	2	0.65	0.74	-0.88	0.48
1	7	3	3.01	2.82	-0.21	-0.98
2	7	3	5.10	4.86	0.26	-0.96
3	7	3	5.46	4.83	0.84	-0.54
4	7	3	0.84	1.08	-0.28	-0.96
5	7	3	2.51	2.44	-0.61	-0.79
7	7	3	0.54	1.16	-0.25	-0.97
1	7	4	3.51	3.63	0.95	0.30
2	7	4	0.84	0.89	0.95	0.32
3	7	4	1.14	1.34	0.73	0.68
4	7	4	1.05	0.94	-0.82	0.57
5	7	4	1.06	1.06	0.52	-0.86
6	7	4	0.62	0.65	0.96	-0.27
1	7	5	1.05	1.05	-0.99	-0.14
2	7	5	1.00	1.06	-0.71	-0.70
1	7	6	0.71	0.88	1.00	-0.04
2	7	6	0.75	0.97	-0.24	-0.98
0	8	0	7.16	7.09	-1.00	0.00
2	8	0	5.22	4.85	-1.00	0.00
3	8	0	2.99	2.91	0.00	1.00
4	8	0	3.51	3.36	-1.00	0.00
6	8	0	1.15	1.42	1.00	0.00
0	8	1	2.75	3.03	-1.00	0.00
1	8	1	3.29	3.69	0.24	-0.97
2	8	1	1.84	1.97	-0.77	-0.63
3	8	1	1.66	1.63	-0.77	-0.63
4	8	1	2.90	3.23	-0.65	0.76
5	8	1	1.64	1.62	0.73	-0.68
6	8	1	1.12	1.27	0.97	-0.24
0	8	2	4.23	4.56	1.00	0.00
1	8	2	2.27	2.83	-0.91	0.42
2	8	2	1.07	1.19	-0.92	-0.38
3	8	2	2.04	2.28	0.92	-0.40
4	8	2	2.68	2.61	0.28	0.96
6	8	2	1.25	1.55	1.00	0.07
0	8	3	3.26	3.28	-1.00	0.00
1	8	3	1.62	1.68	0.76	0.65
2	8	3	1.47	1.76	-0.61	-0.79
3	8	3	2.54	2.68	-0.73	0.69
4	8	3	1.87	2.27	-0.33	0.94
6	8	3	0.57	0.74	1.00	-0.03
0	8	4	1.93	2.37	1.00	0.00
1	8	4	1.36	1.32	-0.05	1.00
2	8	4	2.22	2.38	-0.61	0.79
5	8	4	0.96	0.74	0.95	0.32
3	8	5	1.16	0.95	0.61	0.79
4	8	5	1.20	1.32	0.43	0.91
5	9	0	2.17	2.79	0.00	-1.00
0	9	1	1.43	1.64	0.00	-1.00
1	9	1	2.04	2.15	-0.01	1.00
2	9	1	2.95	2.27	-0.79	-0.62
3	9	1	3.36	3.01	0.78	-0.62
0	9	2	2.19	2.28	0.00	-1.00
1	9	2	2.71	2.35	0.99	-0.16
2	9	2	3.15	3.09	-0.58	-0.81
3	9	2	3.14	3.15	0.79	-0.61
0	9	3	3.01	3.24	0.00	-1.00
1	9	3	2.12	2.49	0.95	0.31
2	9	3	2.10	2.27	0.32	0.95
2	10	0	4.34	4.35	-1.00	0.00
3	10	0	3.66	4.04	0.00	-1.00
1	10	1	2.12	2.30	1.00	0.03
2	10	1	1.52	1.78	0.67	0.74
0	10	2	1.58	1.40	-1.00	0.00
1	10	2	3.15	3.18	0.69	0.73
1	10	3	1.45	1.51	0.54	0.84
1	11	0	2.32	2.21	0.00	-1.00
0	11	1	3.36	3.49	0.00	-1.00
1	11	1	3.66	3.93	0.86	-0.52
0	12	0	4.48	4.60	-1.00	0.00
2	12	1	2.36	2.37	-0.13	0.90
1	12	2	1.38	1.55	-0.80	0.60

This is due to the replacement of the double bond by a single bond.

Packing of molecules

The packing of the molecules also closely resembles that in maleic anhydride, in spite of the additional hydrogen atoms. The closest contacts between the ring oxygen and the carbonyl oxygen are 3·10 and 3·15 Å, oxygen to trigonal carbon contacts vary from 3·02 to 3·34 Å and oxygen to tetrahedral carbon contacts from 3·13 to 3·46 Å, as shown in Fig. 2. Ring oxygen to hydrogen closest contacts are 2·59 Å parallel to the *c* axis

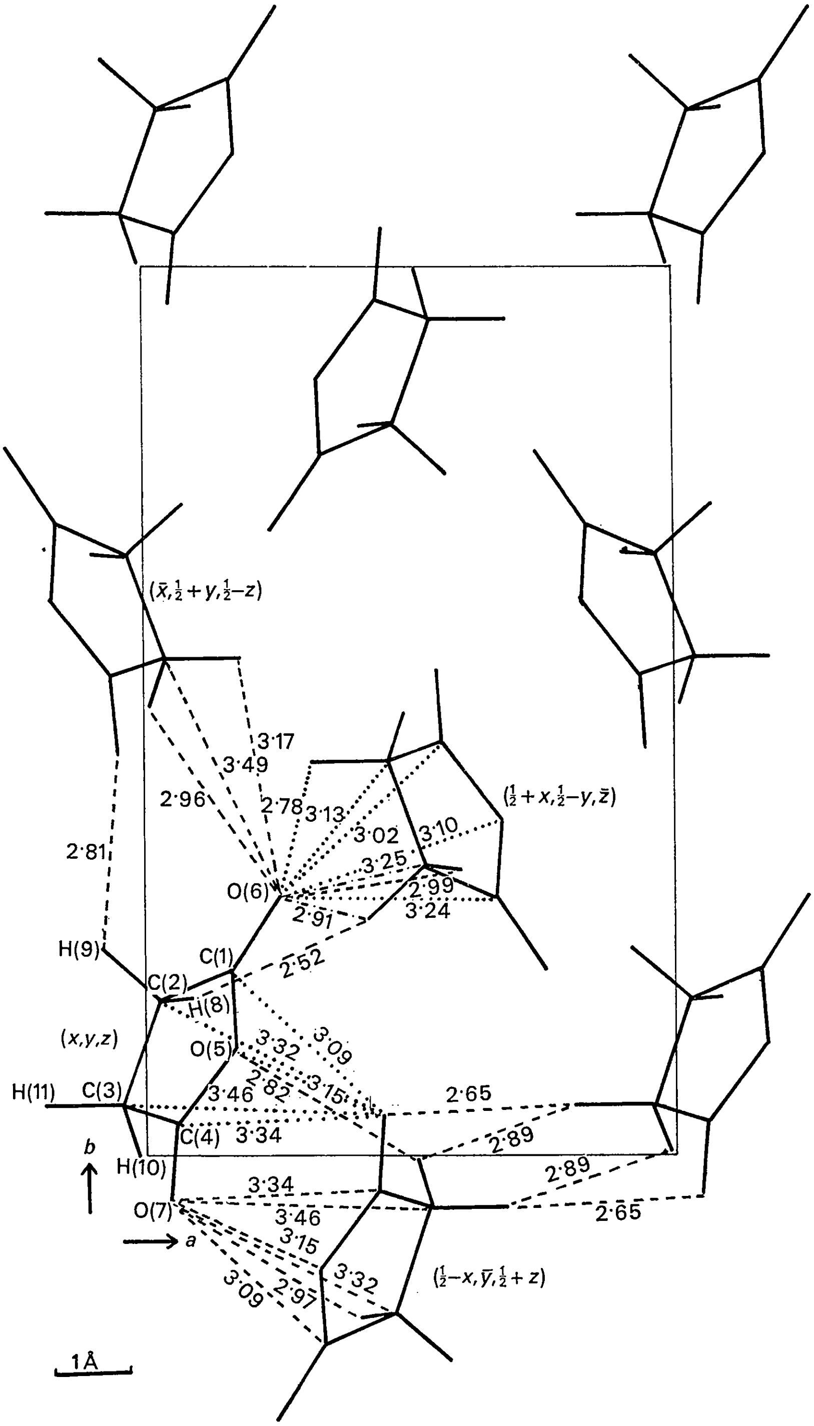

Fig. 2. Intermolecular contacts.
----- contacts to molecule in unit cell of reference molecule
...... contacts to molecules in next cell.

Table 3. *Configuration of succinic anhydride*

Centre of inertia of molecule X_0 = 0·755 Å
Y_0 = 1·457
Z_0 = 2·115

Distance of C(1) from centre of inertia: 1·13 Å
C(4) 1·13
O(5) 0·84

Direction cosines of molecular axes *L*, *M*, *N*.

	a	*b*	*c*
L	0·32466	0·90454	−0·27641
M	0·57387	0·04392	0·81777
N	0·75184	−0·42411	−0·50483

Deviations from plane $0·7518x - 0·4241y - 0·5048z = -1·118$

C(1)	−0·003 Å
C(2)	−0·014
C(3)	+0·013
C(4)	+0·001
O(5)	−0·009
O(6)	+0·010
O(7)	+0·001

and the closest carbonyl oxygen to hydrogen is 2·74 Å, also parallel to the *c* axis.

Temperature factors

All temperature factors in succinic anhydride have lower values than in maleic anhydride. This may be attributed to the additional hydrogen contacts. Table 4 gives the temperature parameters *B* with respect to their vibration ellipsoid axes and the direction cosines of these axes with respect to the crystallographic axes. Table 5 lists corresponding vibration ellipsoid axes in the direction of the molecular axes *L*, *M* and *N*.

The vibration ellipsoids of the carbonyl oxygen atoms have their shortest axes ($B_{\min}$) nearly parallel to the direction of the C=O bonds. The other two axes for O(6) are of lengths B = 6·86, 6·51 and for O(7) B = 7·52, 5·85 respectively. The first two are too nearly equal for their computed directions to have much significance, but the shorter 5·85 axis for O(7) is nearly along [100], which is the direction of the closest ap-

Table 4. *Principal temperature factors, B_i, and their direction cosines with respect to the crystallographic axes*

		B_i	cos α	cos β	cos γ
C(1)	1	4·67	0·0296	0·8655	−0·4999
	2	3·64	0·6184	0·3771	0·6895
	3	3·24	0·7854	−0·3296	−0·5241
C(2)	1	4·72	−0·2826	0·9572	0·0622
	2	4·24	0·8627	0·2820	−0·4199
	3	2·57	0·4195	0·0650	0·9054
C(3)	1	5·21	0·0488	0·9723	−0·2286
	2	3·65	0·8457	−0·1620	−0·5085
	3	2·67	0·5314	0·1686	0·8302
C(4)	1	5·39	0·6274	0·6581	0·4164
	2	3·49	−0·1214	−0·4455	0·8870
	3	3·04	0·7692	−0·6070	−0·1997
O(5)	1	5·12	0·1205	0·9752	−0·1855
	2	3·39	0·8285	−0·2018	−0·5224
	3	2·94	0·5469	0·0908	0·8323
O(6)	1	6·86	0·4478	−0·7201	0·5301
	2	6·51	−0·6464	0·1490	0·7484
	3	3·89	0·6178	0·6777	0·3987
O(7)	1	7·52	0·3279	0·7301	0·5996
	2	5·85	0·9077	−0·0674	−0·4143
	3	4·60	0·2621	−0·6801	0·6847

Table 5. *Temperature factors B_L, B_M, B_N in directions of molecular axes L, M, N*

	B_L	B_M	B_N
C(1)	4·53	3·77	3·25
C(2)	4·51	2·63	4·40
C(3)	5·07	2·71	3·75
C(4)	4·35	4·47	3·09
O(5)	5·02	2·95	3·49
O(6)	5·36	5·34	6·55
O(7)	5·81	6·12	6·05

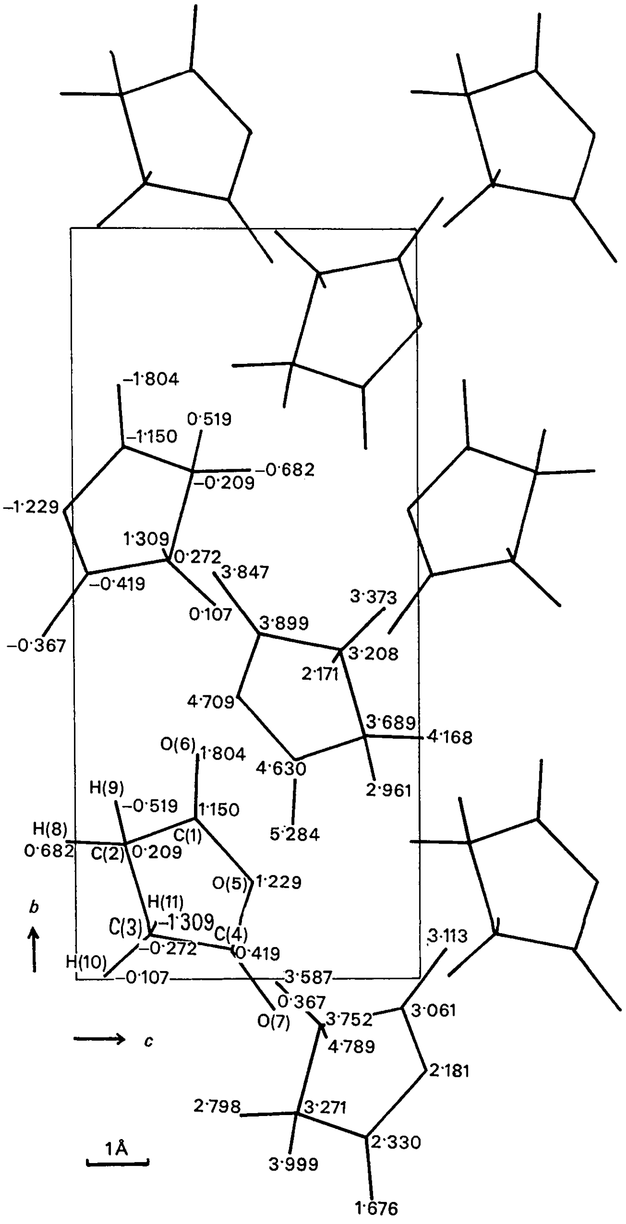

Fig. 3. Projection of structure along [*a*].

proach of the (xyz) and $(\frac{1}{2}-x,\bar{y},\frac{1}{2}+z)$ molecules. It is not surprising that there should be no approximate mirror symmetry of the thermal vibration of the atoms in the molecule, because the intermolecular bonding is far from mirror-symmetrical (Fig. 2).

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Descriptive Symbols for Crystal-Structure Types and Homeotypes Based on Lattice Complexes

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After a short historical review, a description of the invariant cubic lattice complexes according to C. Hermann is given. Besides the Bravais lattices only seven cubic lattice complexes and their splitting products into subgroups are needed. The description of variant cubic complexes, with the aid of coordination polyhedra and invariant complexes, is given for space group *Pm*3*m*. A crystal-structure type is symbolized by a list of lattice complexes, each of which is occupied by a set of equivalent atoms or coordination polyhedra.

Introduction

Attempts have been made in the past to develop a satisfactory and comprehensive nomenclature of structure types.

In the *Strukturberichte* (1931–1943) P. P. Ewald and C. Hermann proposed a classification based on chemical composition. The symbol of a structure type consists of a capital letter followed by a number; it is not self-explanatory, and the authors considered this nomenclature to be only a preliminary solution. Later *Structure Reports* (from 1940 on) reported the results of structure determinations without any reference to structural types.

Laves (1930) published a nomenclature which is especially appropriate for A_mB_n compositions but can also be expanded to $A_mB_nC_p$ compositions. The concept of 'connexion' is emphasized. Connexions in one, two, or three dimensions are symbolized by *I*(island), *C*(chain), *N*(net), or *L*(lattice). Besides these 'homogeneous' connexions (between equivalent atoms), 'heterogeneous' connexions (between dissimilar atoms) are also considered and are represented by small letters. In addition, coordination numbers and distances are also specified.

In six papers Wells (1954*a*–1956) discussed 'the geometrical basis of crystal chemistry', using the examples of regular polyhedra and *n*-connected nets. Wells's *n*-connected nets are special cases of lattice complexes.

Frank & Kasper (1958, 1959) described highly coordinated intermetallic compounds by means of 'triangulated coordination shells'. They have shown that these coordination shells have a number of representatives, but the triangulated coordination shells are not the only coordination polyhedra that are known in structures.

In 1957 a report of the Nomenclature Committee of the ASTM proposed a nomenclature for alloy phases. The symbols suggested consist of three parts; the first one gives the number of atoms in the cell, the last one designates the Bravais lattice by a new letter, and the middle part is a small letter, which distinguishes between different structure types that would otherwise have the same symbol; *e.g.* diamond–8*aF*, NaCl–8*bF*, ZnS(Sph)–8*cF*.

The first edition of the *International Tables (Internationale Tabellen zur Bestimmung von Kristallstrukturen*, 1935) included a good treatment of lattice complexes. C. Hermann redefined the concept, which had been introduced by P. Niggli. Each space-group description