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The Crystal and Molecular Structure of the DL Form of Pentane-2,4-diol Diacetate, $CH_3CH(OCOCH_3)CH_2CH(OCOCH_3)CH_3$

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The DL form of pentane-2,4-diol diacetate, $C_9O_4H_{16}$, crystallizes in space group $P2_1/c$ with 8 molecules in a unit cell of dimensions $a=8{\cdot}24$, $b=27{\cdot}53$, $c=11{\cdot}24$ Å, $\beta=120{\cdot}75°$. Measurement of intensities was performed at 10°C with a proportional counter and photographically, Cu $K\alpha$ radiation being used. The crystal structure was solved on the basis of the three-dimensional Patterson function, and refined by a block-diagonal least-squares procedure with individual isotropic temperature coefficients, neglecting hydrogen atoms. The final R value was 0·234 for 993 observed and about 1092 unobserved reflexions and 0·185 for 993 observed reflexions.

Two independent molecules are of the same conformation within limits of observational errors. Interatomic vectors and angles show no significant deviation from standard values. The acetate groups of the molecule are planar, but not coplanar, their interplanar angle being about 51°. The pentane chain seems to be slightly twisted.

Introduction

The structure of the DL form of pentane-2,4-diol diacetate, the first member of the homologous series of oligomers of polyvinyl acetate, has been solved. The synthesis and separation of this compound was described earlier by Lím and collaborators (Lím, Votavová, Štokr & Petránek, 1965; Lím, Kolínský, Votavová, Ryska & Lukáš, 1965).

Since there is no reason to expect the presence of anomalous interatomic distances in this compound, a moderate level of accuracy was adopted for the structure analysis. The aim of this work is to determine the conformation of the molecules of pentanediol diacetate, and their mutual packing in the crystal.

Experimental

Plate-like, well-developed colourless crystals were easily grown from the melt by slow cooling. The most prominent face is (010). A single-crystal plate approximately 0·6 mm thick was cleaved into prismatic fragments (with dimensions $0{\cdot}6\times0{\cdot}6\times2$ mm) convenient for intensity measurements. As the rate of sublimation of pentanediol diacetate on exposure to air is rather high, the crystals were enclosed in thin-walled capillaries of polymethyl methacrylate (wall thickness 0·1 mm). Specimens thus protected were stable for several months. Lattice constants were calculated from the measurements of the diffraction angles on the diffractometer; the systematic extinctions were determined from the Weissenberg patterns.

Crystal data

DL form of pentane-2,4-diol diacetate, $C_9O_4H_{16}$
m.p. *ca.* 23°C (not measured in this work)

Monoclinic
$a=8{\cdot}24\pm0{\cdot}02$, $b=27{\cdot}53\pm0{\cdot}07$, $c=11{\cdot}24\pm0{\cdot}03$ Å
$\beta=120{\cdot}75\pm0{\cdot}06°$
$U=2191{\cdot}6$ Å^3
$D_x=1{\cdot}142$ g.cm^{-3}, $Z=8$, D_m not measured
$F(000)=816$
Absent spectra: $h0l$ when l is odd
$0k0$ when k is odd
Space group: unambiguously $P2_1/c$

Intensity data

The measurements of intensities were performed at 10°C with Ni-filtered Cu $K\alpha$ radiation. The Weissenberg equiinclination multiple-film technique was combined with measurements on the counter diffractometer in the normal beam arrangement. Different crystals were used and the intensities were measured in two orientations, one with the rotation axis **a**, and the other with **c**. For measurements on the diffractometer, the proportional counter with pulse height analyser was used, and intensities of reflexions on layer lines with $h=0,1,2,3,4$, and $l=0,1,2,3$ were determined. The multiple-film technique was used for layer lines with $h=0,1,2,3,4,5$ and $l=0,1,2,3,4,5,6$. The intensities of reflexions not measured on the diffractometer were estimated visually by comparison of the blackening of their spots on Weissenberg films with the blackening of spots of reflexions whose intensities had been measured on the diffractometer. Care was taken to compare reflexions of the same size and having approximately the same background. The same crystals were used for the Weissenberg and the counter method. 993 nonzero independent reflexions were measured. The zero value of intensity was attributed to reflexions according to Weissenberg photographs. Lorentz and polarization factors were applied and the structure factors derived.

No corrections for absorption and extinction were used. The structure factors were placed on the absolute scale by means of a Wilson plot and at the same time the overall temperature factor was determined, $B=5{\cdot}27$ Å^2.

Solution of the structure

The starting point for the solution of the structure was the fact that of the $0k0$ reflexions present only those with $k=4n$ are very strong. This indicates that the molecules are arranged in four equidistant layers situated at odd or even eighths of the period b. The analysis of maxima on Harker line $(0, y, \frac{1}{2})$ eliminated the first possibility. Eight molecules of DL-pentane-2,4-diol diacetate are thus distributed among four layers, every layer containing a pair of enantiomers. Molecules placed at even fourths of b are coupled together with the centres of symmetry, those at odd fourths of b with glide planes. The approximate orientation of molecules and intermolecular vectors was found from the analysis of a three-dimensional Patterson function, especially from the section at $y=0$, $\frac{1}{4}$ and $\frac{1}{2}$.

In this way approximate coordinates of the carbon and the oxygen atoms were derived and structure factors $F(hk0)$, $F(0kl)$ and $F(h0l)$ with $|h|\leq 5$, $0\leq k\leq 12$, $0\leq l\leq 6$ were calculated. The R values with these input coordinates were 0·34, 0·42 and 0·80 respectively.

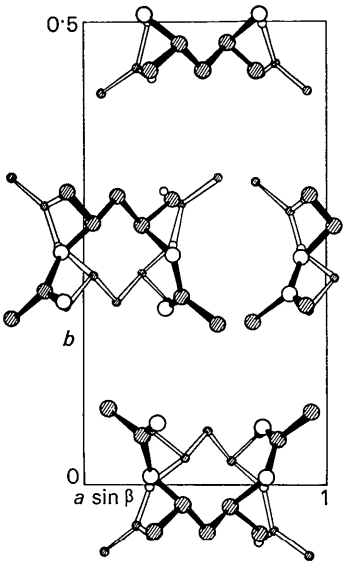

Fig. 1. Projection of the structure along the c axis. Atoms of z coordinate less than 0·5, large circles; atoms of z-coordinate more than 0·5, small circles. Open circles: oxygen atoms; shaded circles: carbon atoms. Molecules at $y=0$ are related through a centre of symmetry at (0·5, 0, 0·5), molecules at $y=0{\cdot}25$ are related through a glide plane (x, 0·25, z).

The refinement

Figs. 1, 2, 3 and 4 showing the final structure explain the relatively low R value ($R=\Sigma\,||F_{obs}|-|F_{calc}||/$

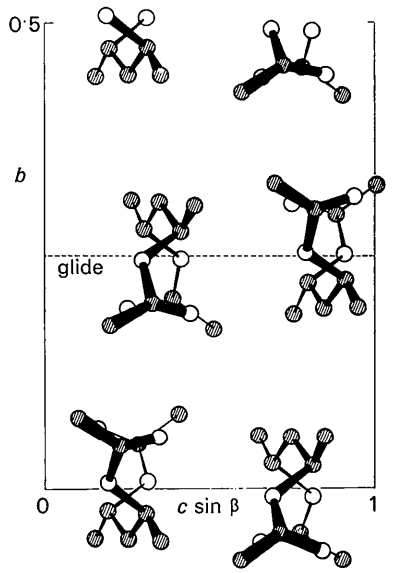

Fig. 2. Projection of the structure along the a axis.

Table 1. *Progress of refinement*

Method	Zones	Damping factor	$R(hkl)$	Note
3-D Fourier	all observed	—	0·551	
3-D Fourier	all observed	—	0·538	Nitrogen atoms
LS-procedure	A		0·445	
	A	0·25	0·419	
	A	0·666	0·382	
	A	0·75	0·355	
	A	0·666	0·340	
	A	0·666	0·318	
	A	0·75	0·294	
	A	1·00	0·244	
	A	1·00	0·219	
	A	1·00	0·212	
	A	1·00	0·210	
	$A+B$	0·5	0·247	
	$A+B$	0·5	0·230	Individual
	$A+B+C+D$	0·666	0·247	isotropic
	$A+B+C+D$	0·75	0·237	temperature
	$A+B+C+D$	1·00	0·235	factor
	$A+B+C+D$	1·00	0·234	

$\Sigma |F_{obs}|$) for $hk0$ and $0kl$ reflexions and the disagreement for the $h0l$ reflexions. In projections along the a and c axes atoms largely overlap, and if the intermolecular vectors are correct the R index can be expected to be relatively low even when the conformation of the molecules is not free of errors. The structure factors of lower orders do not depend in this case very strongly on the 'fine structure' of complex maxima on the projection of the electron density. The projection along the b axis, on the other hand, is quite sensitive to the conformation of the molecule, as the coalescence of electron density maxima is much less important. A number of models were tried and some of them were refined in two dimensions by the least-squares method. The best results were obtained with a model with planar acetate groups, the angle between which was 30°. Here, after several cycles of least-squares refinement (damping factor 0·25) R values decreased to 0·396, 0·314 and 0·294 for $hk0$, $0kl$ and $h0l$ zones respectively. Output coordinates resulting from this calculation were used for the determination of signs of structure factors. With these the three-dimensional electron density function was calculated. The overall R index at this stage was 0·551 for observed reflexions. From the resulting electron density maps it was not possible to decide between two possible orientations (Fig. 5) of the acetate group. The signs for the next three-dimensional electron density function were thus calculated for the model in which the atoms in the acetate groups were averaged over both possible orientations. This means that atoms C(8) and O(3), C(9) and O(4), C(17) and O(7), C(18) and O(8) were replaced by nitrogen atoms equidistant from the atoms C(6) and C(7), C(15) and C(16) respectively. (For numbering of atoms see Fig. 6). The resulting three-dimensional electron density clearly favoured the case in Fig. 5(*a*) (carbonyl oxygen atoms – O(3), O(4), O(7), O(8) in, methyl groups with C(8), C(9), C(17), C(18) out). The coordinates of atoms, derived from this last Fourier synthesis, served as input coordinates for the three-dimensional least-squares block-diagonal refinement. The course of the refinement is summarized in Table 1. For computational convenience, the reflexions were grouped into four zones (Table 2). In the first 11 cycles coordinates and only overall temperature coefficient were refined; from the 12th cycle the individual temperature coefficients were also refined. The refinement was stopped after the 17th cycle, when for most atoms the shifts in coordinates dropped below one-third of their standard deviations. In the calculations, the scattering factors of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for C and O atoms were used. It was not possible in this work to take into account the 16 hydrogen atoms in each molecule, which would have a significant effect on the refinement of the structure. Unobserved reflexions were introduced with one-half the minimum observed struc-

Table 2. *Distribution of reflexions in zones in the least-squares refinement*

Zone	Number of reflexions Observed	Unobserved
A	382	355
B	336	357
C	203	380
D	72	—

Table 3. *Final positional (fractional) and thermal parameters B* with their standard deviations*

	x	y	z	B	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	$\sigma(B)$
C(1)	0·2818	−0·0583	0·3518	5·6644	0·0018	0·0005	0·0013	0·3485
C(2)	0·3986	−0·0275	0·3085	3·9902	0·0015	0·0004	0·0011	0·2705
C(3)	0·5026	−0·0556	0·2497	4·4289	0·0017	0·0005	0·0012	0·2755
C(4)	0·6013	−0·0252	0·1933	4·3170	0·0016	0·0005	0·0012	0·2875
C(5)	0·7184	−0·0542	0·1503	5·4647	0·0018	0·0005	0·0013	0·3348
C(6)	0·2156	0·0457	0·2261	4·8821	0·0017	0·0005	0·0013	0·3124
C(7)	0·7555	0·0494	0·2787	6·1379	0·0019	0·0006	0·0014	0·3695
C(8)	0·0684	0·0738	0·1037	5·6496	0·0018	0·0005	0·0013	0·3451
C(9)	0·9072	0·0785	0·4046	7·4464	0·0021	0·0006	0·0016	0·4408
C(10)	0·6506	0·1958	0·9580	6·0197	0·0019	0·0006	0·0014	0·3662
C(11)	0·7618	0·2256	0·9085	4·1825	0·0016	0·0005	0·0011	0·2798
C(12)	0·8585	0·1936	0·8527	4·4681	0·0016	0·0005	0·0012	0·2900
C(13)	0·9629	0·2228	0·7965	4·2443	0·0016	0·0005	0·0012	0·2796
C(14)	1·0736	0·1886	0·7574	5·1973	0·0017	0·0005	0·0013	0·3304
C(15)	0·5929	0·3007	0·8238	5·5160	0·0018	0·0005	0·0013	0·3357
C(16)	1·1579	0·2945	0·8850	5·8506	0·0018	0·0005	0·0014	0·3548
C(17)	0·4542	0·3285	0·6981	5·8241	0·0019	0·0006	0·0014	0·3632
C(18)	1·2949	0·3246	1·0078	5·1674	0·0017	0·0005	0·0013	0·3284
O(1)	0·2614	0·0040	0·1926	3·2625	0·0009	0·0003	0·0007	0·1591
O(2)	0·7312	0·0056	0·3094	4·4473	0·0010	0·0003	0·0008	0·1908
O(3)	0·2731	0·0579	0·3461	6·7501	0·0013	0·0004	0·0010	0·2656
O(4)	0·7006	0·0641	0·1578	8·3816	0·0015	0·0004	0·0011	0·3178
O(5)	0·6303	0·2566	0·7938	4·1016	0·0010	0·0003	0·0007	0·1802
O(6)	1·1030	0·2532	0·9106	4·1560	0·0010	0·0003	0·0007	0·1848
O(7)	0·6641	0·3142	0·9432	7·7453	0·0014	0·0004	0·0010	0·2967
O(8)	1·0873	0·3070	0·7581	7·0723	0·0013	0·0004	0·0010	0·2797

* The temperature factor here is defined as $\exp\{-B\sin^2\theta/\lambda^2\}$.

Table 4. *Measured and calculated structure factors*

The values listed are h, k, l, $|F_o|$ and F_c; unobserved reflexions are listed as $|F_o| = 3{\cdot}05$.

1	0	0	20.53	-16.00
2	0	0	99.51	-102.02
3	0	0	51.62	51.55
4	0	0	3.05	5.40
5	0	0	31.86	-29.31
6	0	0	33.64	-27.37
7	0	0	3.05	0.63
8	0	0	12.23	7.96
-9	0	2	15.37	14.32
-8	0	2	15.52	-11.98
-7	0	2	3.05	2.31
-6	0	2	41.44	40.83
-5	0	2	3.05	2.02
-4	0	2	41.89	-38.72
-3	0	2	45.99	28.30
-2	0	2	3.05	-1.07
-1	0	2	44.27	42.91
0	0	2	169.64	-185.05
1	0	2	7.33	7.52
2	0	2	3.05	-2.33
3	0	2	3.05	-2.76
4	0	2	11.20	-13.54
5	0	2	13.16	-12.84
6	0	2	3.05	4.15
-9	0	4	7.42	-8.03
-7	0	4	15.24	-15.29
-6	0	4	5.87	6.30
-5	0	4	3.05	-4.86
-4	0	4	29.91	38.88
-3	0	4	5.72	7.44
-2	0	4	3.05	0.88
-1	0	4	17.31	-27.42
0	0	4	3.05	-3.46
1	0	4	16.69	-16.28
2	0	4	42.22	39.74
3	0	4	3.05	1.81
4	0	4	3.05	-1.54
5	0	4	12.47	9.04
6	0	4	3.05	0.12
-5	0	6	13.38	20.43
-4	0	6	21.39	42.36
-3	0	6	3.05	-3.99
-2	0	6	73.69	-84.31
-1	0	6	18.37	17.48
0	0	6	3.05	6.02
1	0	6	69.63	-68.92
2	0	6	3.05	-7.57
3	0	6	22.26	27.20
-5	0	8	45.04	-51.20
-4	0	8	3.05	-6.22
-3	0	8	10.11	8.82
-2	0	8	23.56	20.87
-1	0	8	3.05	0.97
0	0	8	8.04	-14.02
1	0	8	10.65	25.69
2	0	8	3.05	-0.81
3	0	8	24.81	-16.31
-5	0	10	7.94	9.67
-4	0	10	3.05	-2.01
-3	0	10	3.05	6.22
0	0	10	12.69	10.79
3	0	10	3.05	0.67
-4	0	12	12.70	11.80
-3	0	12	23.48	-12.70
1	1	0	43.90	35.46
2	1	0	100.68	-101.62
3	1	0	15.16	-16.91
4	1	0	3.05	-5.99
5	1	0	9.87	-16.45
6	1	0	16.67	17.90
7	1	0	3.05	-0.30
-7	1	1	3.05	-1.20
-6	1	1	3.05	2.10
-5	1	1	8.84	10.44
-4	1	1	8.69	-8.53
-3	1	1	3.05	-2.93
-2	1	1	48.90	42.30
-1	1	1	omitted	
0	1	1	14.56	-13.16
1	1	1	3.05	-3.99
2	1	1	3.05	-8.31
3	1	1	3.05	-1.86
4	1	1	3.05	6.79
5	1	1	3.05	-2.31
6	1	1	3.05	-1.04
7	1	1	3.05	-1.38
-8	1	2	15.53	14.23
-7	1	2	3.05	-2.88
-6	1	2	3.05	0.44
-5	1	2	3.05	-8.61
-4	1	2	41.97	-42.32
-3	1	2	11.56	-8.21
-2	1	2	51.49	-42.25
-1	1	2	28.01	28.37
0	1	2	135.79	133.63
1	1	2	31.99	28.45
2	1	2	3.05	-1.92
3	1	2	3.05	1.33
4	1	2	12.76	-16.60
5	1	2	3.05	4.05
6	1	2	3.05	-2.96
-7	1	3	3.05	-0.12
-6	1	3	3.05	-3.29
-5	1	3	8.97	8.61
-4	1	3	3.05	1.28
-3	1	3	3.05	-7.35
-2	1	3	3.05	-3.39
-1	1	3	3.05	-1.49
0	1	3	16.59	-13.17
1	1	3	3.05	-0.95
2	1	3	3.05	-2.41
3	1	3	3.05	-0.25
4	1	3	3.05	-2.71
5	1	3	3.05	1.23
6	1	3	3.05	-0.88
-7	1	4	6.54	-4.21
-6	1	4	5.88	-5.62
-5	1	4	4.98	-3.92
-4	1	4	5.32	9.64
-3	1	4	11.42	-13.09
-2	1	4	3.05	-5.83
-1	1	4	3.05	4.84
0	1	4	17.68	9.30
1	1	4	7.59	-11.98
2	1	4	16.55	-17.63
3	1	4	3.05	-4.44
4	1	4	3.05	0.53
5	1	4	12.47	-10.49
6	1	4	3.05	1.70
-7	1	5	3.05	1.62
-6	1	5	3.05	6.48
-5	1	5	3.05	-2.36
-4	1	5	3.05	-3.90
-3	1	5	7.72	-7.46
-2	1	5	3.05	-1.23
-1	1	5	7.28	-5.82
0	1	5	3.05	2.77
1	1	5	3.05	3.79
2	1	5	3.05	2.90
3	1	5	3.05	-4.19
4	1	5	3.05	1.43
5	1	5	3.05	1.29
6	1	5	3.05	-0.95
-5	1	6	12.03	11.46
-4	1	6	17.84	-21.14
-3	1	6	3.05	-1.78
-2	1	6	18.45	-27.87
-1	1	6	18.39	-16.54
0	1	6	9.65	14.75
1	1	6	3.05	-0.76
2	1	6	14.94	18.76
3	1	6	22.27	30.47
-4	1	7	8.36	-15.42
-3	1	7	3.05	1.80
-2	1	7	3.05	2.55
-1	1	7	3.05	-2.18
0	1	7	3.05	-3.96
1	1	7	3.05	3.10
2	1	7	3.05	2.45
3	1	7	3.05	0.15
-4	1	8	18.11	18.82
-3	1	8	10.12	7.53
-1	1	8	3.05	6.69
0	1	8	8.04	-12.14
1	1	8	10.65	-16.74
3	1	8	3.05	-4.36
-4	1	9	3.05	2.37
-3	1	9	3.05	0.53
0	1	9	3.05	1.63
3	1	9	3.05	-0.40
-5	1	10	7.94	-8.41
-4	1	10	3.05	-4.77
-4	1	11	3.05	4.22
-4	1	12	12.70	-9.93
0	2	0	3.05	0.88
1	2	0	83.08	-70.60
2	2	0	95.05	-94.78
3	2	0	3.05	5.63
4	2	0	74.10	72.92
5	2	0	3.05	-4.52
6	2	0	16.69	-15.17
7	2	0	6.46	8.17
-7	2	1	3.05	-0.62
-6	2	1	12.04	10.70
-5	2	1	8.84	7.43
-4	2	1	3.05	2.12
-3	2	1	23.17	25.60
-2	2	1	22.26	22.62
-1	2	1	16.27	-16.14
0	2	1	53.19	-57.32
1	2	1	3.05	2.36
2	2	1	9.35	20.53
3	2	1	21.87	-19.84
4	2	1	3.05	-1.28
5	2	1	3.05	-4.95
6	2	1	3.05	1.82
7	2	1	3.05	2.10
-8	2	2	15.53	-13.27
-7	2	2	3.05	-9.10
-6	2	2	3.05	0.25
-5	2	2	17.05	17.78
-4	2	2	42.23	-44.20
-3	2	2	3.05	-2.09
-2	2	2	219.26	237.89
-1	2	2	14.30	12.94
0	2	2	92.96	-93.04
1	2	2	116.32	96.19
2	2	2	3.05	3.32
3	2	2	3.05	-0.73
4	2	2	25.07	-27.57
5	2	2	3.05	1.12
6	2	2	12.65	9.96
-9	2	3	12.81	6.14
-7	2	3	8.72	7.32
-6	2	3	3.05	-6.38
-5	2	3	3.05	-1.77
-4	2	3	16.00	18.77
-3	2	3	8.84	-21.62
-2	2	3	3.05	-3.08
-1	2	3	51.59	-30.94
0	2	3	21.08	-14.80
1	2	3	3.05	2.49
2	2	3	37.04	-37.84
3	2	3	3.05	1.43
4	2	3	3.05	2.20
5	2	3	9.47	9.74
6	2	3	3.05	-1.07
-8	2	4	16.52	15.14
-7	2	4	[illegible]	[illegible]
-6	2	4	[illegible]	[illegible]
-5	2	4	7.93	5.84
-4	2	4	3.05	-3.00
-3	2	4	28.92	28.38
-2	2	4	14.63	-15.05
-1	2	4	3.05	-1.78
0	2	4	32.56	-18.32
1	2	4	3.05	-2.87
2	2	4	3.05	5.70
3	2	4	70.08	-70.20
4	2	4	3.05	3.78
5	2	4	12.50	11.93
6	2	4	3.05	-1.80
-7	2	5	7.35	-6.60
-6	2	5	3.05	5.64
-5	2	5	3.05	-1.79
-4	2	5	16.60	-27.87
-3	2	5	3.05	1.23
-2	2	5	3.05	-3.31
-1	2	5	16.07	-10.49
0	2	5	3.05	0.67
1	2	5	10.39	-12.91
2	2	5	17.59	12.22
3	2	5	3.05	1.68
4	2	5	10.33	12.49
5	2	5	3.05	-1.30
6	2	5	3.05	-0.27
-5	2	6	9.93	10.24
-4	2	6	6.95	9.39
-3	2	6	51.58	-51.60
-2	2	6	9.10	-9.49
-1	2	6	20.76	21.12
0	2	6	53.70	37.85
1	2	6	3.05	-0.09
2	2	6	35.01	-27.89
3	2	6	22.27	32.07
-4	2	7	8.44	-12.69
-3	2	7	3.05	1.57
-2	2	7	10.39	2.97
-1	2	7	3.05	-2.25
0	2	7	3.05	3.36
1	2	7	24.44	20.38
2	2	7	3.05	-2.22
3	2	7	3.05	1.93
-4	2	8	18.16	-18.82
-3	2	8	10.21	8.31
-2	2	8	3.05	1.56
-1	2	8	27.71	-29.27
1	2	8	10.65	11.24
2	2	8	16.86	14.68
3	2	8	3.05	-2.22
-4	2	9	3.05	0.91
-3	2	9	3.05	-3.06
-1	2	9	3.05	-1.50
1	2	9	3.05	-1.72
2	2	9	3.05	-1.30
3	2	9	3.05	-1.42
-4	2	10	14.58	-15.88
-3	2	10	3.05	2.61
3	2	10	3.05	-0.27
-4	2	11	3.05	-3.36
-3	2	11	22.62	14.44
3	2	11	3.05	-0.56
-4	2	12	12.71	7.46
-3	2	12	3.05	-4.80
1	3	0	31.70	-25.82
2	3	0	71.20	66.89
3	3	0	12.53	12.77
4	3	0	3.05	7.87
5	3	0	3.05	-2.47
6	3	0	16.71	-17.30
7	3	0	3.05	-2.03
-7	3	1	3.05	-2.64
-6	3	1	12.06	10.54
-5	3	1	6.89	-3.58
-4	3	1	3.05	-2.49
-3	3	1	3.05	3.27
-2	3	1	48.62	-47.55
-1	3	1	26.51	-28.77
0	3	1	16.84	21.93
1	3	1	12.01	6.57
2	3	1	8.30	13.32
3	3	1	20.95	22.56
4	3	1	3.05	-4.76
5	3	1	3.05	-4.89
6	3	1	7.50	-5.01
7	3	1	3.05	4.96
-8	3	2	15.55	-3.71
-7	3	2	3.05	5.18
-6	3	2	3.05	-4.49
-5	3	2	6.12	6.22
-4	3	2	30.59	34.22
-3	3	2	26.22	-27.81
-2	3	2	3.05	3.18
-1	3	2	21.39	-26.88
0	3	2	100.47	-102.26
1	3	2	15.53	-10.05
2	3	2	9.92	-4.66
3	3	2	3.05	7.11
4	3	2	11.65	11.04
5	3	2	3.05	-3.09
6	3	2	3.05	3.81
-7	3	3	8.73	9.91
-6	3	3	3.05	-1.85
-5	3	3	6.85	-9.07
-4	3	3	20.54	30.31
-3	3	3	5.87	11.06
-2	3	3	26.10	-26.34
-1	3	3	9.09	-0.96
0	3	3	35.01	24.93
1	3	3	3.05	7.38
2	3	3	3.05	6.53
3	3	3	3.05	-4.10
4	3	3	3.05	-0.41
5	3	3	5.70	-7.93
6	3	3	3.05	3.68
-7	3	4	3.05	2.92
-6	3	4	9.38	7.64
-5	3	4	5.66	-5.10
-4	3	4	9.84	-15.69
-3	3	4	36.51	32.49
-2	3	4	14.97	13.75
-1	3	4	10.04	-7.31
0	3	4	3.05	3.18
1	3	4	16.79	-11.29
2	3	4	16.75	14.25
3	3	4	3.05	0.84
4	3	4	3.05	-3.61
5	3	4	12.53	11.27
6	3	4	3.05	1.81
-7	3	5	7.37	7.45
-6	3	5	8.87	-11.89
-5	3	5	12.76	-10.77
-4	3	5	3.05	4.92
-3	3	5	3.05	2.86
-2	3	5	7.96	-14.18
-1	3	5	7.45	4.49
0	3	5	3.05	-0.80
1	3	5	9.99	-9.25
2	3	5	15.69	-15.77
3	3	5	3.05	3.44
4	3	5	3.05	1.26
5	3	5	3.05	2.19
6	3	5	3.05	-0.95
-5	3	6	12.50	-12.12
-4	3	6	18.33	15.33
-3	3	6	3.05	4.77
-2	3	6	17.28	18.92
-1	3	6	20.92	19.37
0	3	6	9.74	-12.22
1	3	6	3.05	2.35
2	3	6	15.02	-12.19
3	3	6	22.32	-18.25
-4	3	7	4.75	8.47
-3	3	7	3.05	1.60
-2	3	7	3.05	5.81
-1	3	7	3.05	4.24
0	3	7	3.05	0.84
1	3	7	3.05	-7.13
2	3	7	3.05	2.80
3	3	7	3.05	4.02
-3	3	8	10.21	-6.10
-1	3	8	3.05	1.75
0	3	8	11.41	14.95
1	3	8	10.65	9.86
3	3	8	3.05	2.71
-3	3	9	3.05	-6.42
0	3	9	3.05	2.65
3	3	9	3.05	-0.71
0	4	0	214.49	211.97
1	4	0	14.23	-11.71
2	4	0	59.51	-54.46
3	4	0	14.69	19.44
4	4	0	3.05	1.48
5	4	0	3.05	4.53
6	4	0	16.74	-17.74
7	4	0	3.05	0.46
8	4	0	12.21	9.60
-7	4	1	3.05	1.73
-6	4	1	3.05	3.20
-5	4	1	6.95	4.69
-4	4	1	18.96	-18.07
-3	4	1	3.05	-4.31
-2	4	1	104.72	113.49
-1	4	1	43.11	-45.19
0	4	1	6.50	-7.19
1	4	1	169.53	-137.94
2	4	1	11.98	15.15
3	4	1	14.63	-14.49
4	4	1	22.60	-22.11
5	4	1	3.05	-0.63
6	4	1	7.50	4.12
7	4	1	3.05	4.80
-9	4	2	15.31	11.80
-7	4	2	3.05	-2.12
-6	4	2	18.52	16.48
-5	4	2	3.05	4.45
-4	4	2	3.05	-7.36
-3	4	2	83.96	-91.97
-2	4	2	3.05	1.88
-1	4	2	37.73	49.47
0	4	2	99.76	-100.70
1	4	2	3.05	2.51
2	4	2	55.84	42.84
3	4	2	14.98	13.65
4	4	2	6.23	-7.74
5	4	2	13.25	-13.27
6	4	2	3.05	2.61
-8	4	3	6.76	-7.35
-7	4	3	8.74	7.59
-6	4	3	3.05	-1.53
-5	4	3	19.42	18.12
-4	4	3	13.45	20.51
-3	4	3	9.93	3.01
-2	4	3	111.36	-109.49
-1	4	3	3.05	2.29
0	4	3	38.60	-27.76
1	4	3	13.68	22.56
2	4	3	3.05	-0.55
3	4	3	12.42	8.57
4	4	3	3.05	2.40
5	4	3	3.05	4.82
6	4	3	3.05	3.09
-6	4	4	9.44	6.22
-5	4	4	3.05	-1.31
-4	4	4	39.01	-29.45
-3	4	4	31.41	28.33
-2	4	4	12.92	-9.90
-1	4	4	65.07	-58.37
0	4	4	3.05	[illegible]
1	4	4	35.17	28.97
2	4	4	16.94	15.00
3	4	4	3.05	-1.00
4	4	4	9.74	12.42
5	4	4	7.95	7.31
6	4	4	3.05	-1.22
-8	4	5	8.68	7.36
-6	4	5	26.97	20.90
-5	4	5	22.66	-25.90
-4	4	5	3.05	1.06
-3	4	5	37.44	-29.93
-2	4	5	8.07	-11.78
-1	4	5	3.05	3.66
0	4	5	11.49	5.56
1	4	5	3.05	-3.67
2	4	5	17.81	15.88
3	4	5	3.05	3.26
4	4	5	3.05	-2.29
5	4	5	13.54	-4.93
6	4	5	3.05	1.66
-5	4	6	14.31	16.31
-4	4	6	19.61	25.95
-3	4	6	3.05	0.85
-2	4	6	3.05	-4.63
-1	4	6	21.15	17.45
0	4	6	3.05	3.85
1	4	6	36.37	-30.48
2	4	6	3.05	-4.80
3	4	6	15.66	12.40
-5	4	7	3.05	1.02
-4	4	7	3.05	-5.16
-3	4	7	13.59	10.52
-2	4	7	3.05	0.74
-1	4	7	13.90	-4.84
0	4	7	3.05	5.10
1	4	7	3.05	0.36
2	4	7	3.05	3.31
3	4	7	3.05	1.59
-5	4	8	13.76	-10.01
-4	4	8	3.05	-2.53
-3	4	8	3.05	2.32
-2	4	8	19.54	23.22
-1	4	8	3.05	-1.16
0	4	8	15.52	-21.59
1	4	8	10.68	9.08
2	4	8	3.05	0.20
3	4	8	17.30	-10.99
-4	4	9	16.16	19.45
-3	4	9	11.22	-6.70
-2	4	9	3.05	3.07
-1	4	9	24.52	19.17
0	4	9	3.05	-2.41
1	4	9	3.05	-3.39
2	4	9	3.05	-1.64
3	4	9	3.05	0.36
-3	4	10	17.36	16.38
-1	4	10	3.05	-1.88
0	4	10	17.28	13.61
1	4	10	3.05	-0.17
3	4	10	3.05	-1.03
-3	4	11	3.05	-1.18
3	4	11	3.05	-1.15
-3	4	12	23.46	14.05
1	5	0	31.80	23.00
2	5	0	46.73	-44.24
3	5	0	3.05	0.25
4	5	0	3.05	2.19
5	5	0	3.05	4.70
6	5	0	3.05	6.09
7	5	0	3.05	1.59
-7	5	1	3.05	-0.82
-6	5	1	7.81	-8.16
-5	5	1	3.05	4.97
-4	5	1	3.05	2.62
-3	5	1	8.33	-10.53
-2	5	1	57.00	59.42
-1	5	1	37.61	43.06
0	5	1	8.77	-12.86
1	5	1	18.14	-14.61
2	5	1	35.78	-36.40
3	5	1	15.03	-12.76
4	5	1	7.68	7.04
5	5	1	3.05	1.69
6	5	1	3.05	1.53
7	5	1	3.05	-2.51
-7	5	2	3.05	-1.64
-6	5	2	3.05	-4.58
-5	5	2	3.05	-7.62
-4	5	2	19.04	13.94
-3	5	2	31.47	32.40
-2	5	2	11.74	16.67
-1	5	2	27.69	33.94
0	5	2	41.52	52.83
1	5	2	10.85	-9.90
2	5	2	10.37	5.38
3	5	2	30.90	-31.96
4	5	2	12.53	-7.62
5	5	2	3.05	-0.54
6	5	2	7.55	-7.97
-7	5	3	8.76	-7.80
-6	5	3	3.05	-0.89
-5	5	3	3.05	-1.01
-4	5	3	29.09	-31.43
-3	5	3	6.52	2.14
-2	5	3	16.63	16.20
-1	5	3	3.05	-4.41
0	5	3	14.26	-11.08
1	5	3	17.98	-22.60
2	5	3	3.05	-2.43
3	5	3	3.05	4.50
4	5	3	3.05	-2.33
5	5	3	5.77	8.46
6	5	3	3.05	-0.04
-7	5	4	6.60	5.06
-6	5	4	6.01	-1.98
-5	5	4	13.28	-16.23
-4	5	4	26.76	-23.08
-3	5	4	52.45	-47.40
-2	5	4	20.89	-19.23
-1	5	4	3.05	5.67
0	5	4	18.18	-14.21
1	5	4	45.54	37.02
2	5	4	3.05	0.73
3	5	4	3.05	-1.36
4	5	4	3.05	6.30
5	5	4	3.05	-2.90
6	5	4	3.05	-3.60
-7	5	5	7.42	-7.61
-6	5	5	9.03	12.15
-5	5	5	15.54	14.88
-4	5	5	3.05	2.15
-3	5	5	3.05	-1.07
-2	5	5	5.90	9.73
-1	5	5	3.05	7.37
0	5	5	3.05	2.97
1	5	5	14.77	12.36
2	5	5	15.92	12.17
3	5	5	3.05	-2.96
4	5	5	3.05	1.37
5	5	5	3.05	-2.08
6	5	5	3.05	-0.64
-5	5	6	14.92	12.78
-4	5	6	9.07	-10.89
-3	5	6	3.05	-3.15
-2	5	6	12.97	12.89
-1	5	6	21.41	-14.78
0	5	6	7.02	11.03
1	5	6	3.05	-1.07
2	5	6	3.05	5.94
3	5	6	15.78	10.16
-5	5	7	3.05	2.30
-4	5	7	4.89	-8.37
-3	5	7	3.05	-3.04
-2	5	7	3.05	-2.91
-1	5	7	9.92	-8.72
0	5	7	3.05	-4.92
1	5	7	3.05	4.84
2	5	7	3.05	0.11
3	5	7	3.05	-2.48
-5	5	8	3.05	4.55
-3	5	8	3.05	2.01
-1	5	8	3.05	1.05
0	5	8	11.48	-12.92
1	5	8	3.05	-1.73
3	5	8	3.05	-2.07
-5	5	9	7.61	-10.38
-3	5	9	11.28	10.05
0	5	9	3.05	-0.70
3	5	9	3.05	-1.03
-3	5	10	3.05	9.06
3	5	10	3.05	0.30
0	6	0	3.05	2.51
1	6	0	62.61	-53.53
2	6	0	19.92	-17.39
3	6	0	3.05	3.12
4	6	0	20.75	7.50
5	6	0	3.05	4.79
6	6	0	3.05	-3.29
7	6	0	6.54	10.08
-7	6	1	3.05	-0.60
-6	6	1	11.04	7.86
-5	6	1	3.05	4.93
-4	6	1	3.05	-1.85
-3	6	1	7.32	15.86
-2	6	1	25.80	24.79
-1	6	1	33.67	-32.24
0	6	1	9.35	-22.13
1	6	1	3.05	-1.12
2	6	1	62.39	66.01
3	6	1	3.05	-5.15
4	6	1	3.05	-1.47
5	6	1	7.18	-4.82
6	6	1	3.05	1.63
7	6	1	3.05	3.23
-7	6	2	3.05	-7.39
-6	6	2	3.05	-0.84
-5	6	2	10.80	13.21
-4	6	2	16.06	13.95
-3	6	2	13.15	-14.48
-2	6	2	51.72	-43.03
-1	6	2	20.19	26.33
0	6	2	16.60	-21.29
1	6	2	97.44	-88.83
2	6	2	3.05	1.02
3	6	2	46.78	46.57
4	6	2	12.25	-12.10
5	6	2	3.05	-0.86
6	6	2	31.59	27.53
-9	6	3	14.00	8.77
-7	6	3	8.78	9.20
-6	6	3	15.30	-18.53
-5	6	3	3.05	-1.72
-4	6	3	21.80	25.21
-3	6	3	11.41	-12.58
-2	6	3	3.05	1.68
-1	6	3	25.05	-17.33
0	6	3	3.05	3.58
1	6	3	20.35	21.97
2	6	3	74.48	-62.51
3	6	3	3.05	2.37
4	6	3	3.05	1.03
5	6	3	6.00	7.09
6	6	3	3.05	-1.14
-8	6	4	16.85	-11.10
-7	6	4	3.05	4.70
-6	6	4	9.61	4.66
-5	6	4	64.86	-72.93
-4	6	4	3.05	2.54
-3	6	4	91.26	86.09
-2	6	4	34.36	-32.89
-1	6	4	3.05	1.81

Table 4 (*cont.*)

0	6	4	55.11	58.10
1	6	4	46.39	37.89
2	6	4	3.05	-3.70
3	6	4	20.62	-19.37
4	6	4	3.05	2.09
5	6	4	3.05	3.52
6	6	4	21.32	-12.95
-7	6	5	10.02	-17.40
-6	6	5	8.12	11.66
-5	6	5	3.05	-1.76
-4	6	5	21.78	-24.87
-3	6	5	3.05	1.33
-2	6	5	3.05	1.48
-1	6	5	12.16	16.12
0	6	5	3.05	-2.46
1	6	5	40.99	-33.96
2	6	5	16.08	15.64
3	6	5	3.05	1.79
4	6	5	10.58	12.46
5	6	5	3.05	-1.62
6	6	5	3.05	-0.51
-5	6	6	17.22	11.89
-4	6	6	4.37	5.78
-3	6	6	50.68	-38.44
-2	6	6	3.05	3.20
-1	6	6	14.41	8.02
0	6	6	21.98	26.29
1	6	6	3.05	-2.84
2	6	6	3.05	-2.61
3	6	6	3.05	4.60
-5	6	7	12.74	15.53
-4	6	7	4.98	-8.69
-3	6	7	3.05	2.38
-2	6	7	8.62	6.23
-1	6	7	3.05	-5.72
0	6	7	3.05	5.13
1	6	7	24.83	17.36
2	6	7	3.05	-1.70
3	6	7	3.05	1.83
-5	6	8	3.05	1.36
-3	6	8	3.05	-2.69
-2	6	8	3.05	1.29
-1	6	8	28.29	31.44
0	6	8	11.52	-11.86
1	6	8	3.05	-1.52
2	6	8	9.27	7.93
3	6	8	3.05	0.30
-5	6	9	7.67	-11.20
-3	6	9	11.35	-9.09
-2	6	9	3.05	1.24
-1	6	9	3.05	-1.43
0	6	9	3.05	1.92
1	6	9	3.05	-1.64
2	6	9	3.05	-1.68
3	6	9	3.05	-0.35
-5	6	10	16.30	-6.58
-4	6	10	11.29	15.89
-3	6	10	3.05	0.34
-2	6	10	11.01	-11.08
-1	6	10	18.66	-17.12
1	6	10	3.05	-3.82
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1	11	6	3.05	1.81
2	11	6	3.05	1.64
-5	11	7	3.05	4.59
-4	11	7	3.05	-3.85
-3	11	7	3.05	-5.48
-2	11	7	3.05	3.14
-1	11	7	15.52	13.79

0	11	7	3.05	2.78
1	11	7	3.05	2.98
2	11	7	3.05	-1.70
-5	11	8	3.05	-1.02
-4	11	8	14.00	-15.09
-3	11	8	11.23	10.44
-1	11	8	3.05	0.87
0	11	8	11.68	8.42
1	11	8	3.05	-3.26
-5	11	9	3.05	-1.73
-3	11	9	3.05	5.38
0	11	9	3.05	-2.08
-5	11	10	26.69	-14.26
-3	11	10	3.05	-5.69
0	12	0	36.02	12.08
1	12	0	3.05	3.52
2	12	0	3.05	-1.24
3	12	0	17.08	16.53
4	12	0	3.05	-0.80
5	12	0	16.69	-18.01
6	12	0	3.05	-7.96
-7	12	1	6.81	-4.50
-6	12	1	3.05	-0.17
-5	12	1	13.61	15.88
-4	12	1	26.86	-27.26
-3	12	1	3.05	1.48
-2	12	1	37.10	-26.50
-1	12	1	8.85	10.22
0	12	1	7.47	7.73
1	12	1	19.45	-14.41
2	12	1	3.05	6.59
3	12	1	9.64	9.51
4	12	1	14.90	-18.19
5	12	1	3.05	2.85
6	12	1	3.05	-4.98
-6	12	2	9.28	-5.80
-5	12	2	6.74	7.18
-4	12	2	3.05	4.78
-3	12	2	38.72	-26.04
-2	12	2	3.05	-2.50
-1	12	2	67.18	56.85
0	12	2	22.31	17.32
1	12	2	3.05	-6.78
2	12	2	19.07	22.52
3	12	2	3.05	1.01
4	12	2	3.05	-6.01
5	12	2	3.05	-5.82
-8	12	3	8.64	-5.15
-6	12	3	3.05	1.60
-5	12	3	24.92	-28.97
-4	12	3	3.05	-6.31
-3	12	3	13.61	-12.12
-2	12	3	55.62	57.97
-1	12	3	3.05	-4.80
0	12	3	3.05	2.79
1	12	3	35.96	28.91
2	12	3	3.05	-1.24
3	12	3	3.05	-3.80
5	12	3	3.05	-1.38
-9	12	4	16.88	-6.96
-7	12	4	27.18	23.03
-6	12	4	10.38	15.82
-5	12	4	3.05	-3.58
-4	12	4	3.05	-7.94
-3	12	4	17.08	17.04
-2	12	4	3.05	3.84
-1	12	4	45.07	-51.19
0	12	4	3.05	-3.76
1	12	4	13.95	11.39
2	12	4	33.37	-35.67
3	12	4	3.05	0.88
-8	12	5	8.44	6.45
-6	12	5	8.78	-5.39
-5	12	5	13.37	17.38
-4	12	5	3.05	1.77
-3	12	5	25.89	24.72
-2	12	5	12.42	7.56
-1	12	5	8.18	6.11
0	12	5	13.58	-11.80
1	12	5	3.05	-0.41
2	12	5	3.05	-0.28
-5	12	6	3.05	3.89
-4	12	6	16.35	25.71
-3	12	6	3.05	-0.88
-2	12	6	34.99	-34.86
-1	12	6	3.05	-0.92
0	12	6	3.05	1.83
1	12	6	10.39	-12.50
2	12	6	3.05	0.57
-5	12	7	3.05	-0.33
-4	12	7	3.05	-4.44
-3	12	7	3.05	-4.28
-2	12	7	3.05	-1.46
-1	12	7	17.54	-21.93
0	12	7	3.05	4.29
1	12	7	3.05	-0.82
2	12	7	3.05	-0.08
-5	12	8	23.89	15.68
-4	12	8	6.07	-8.43
-3	12	8	6.33	-5.89
-2	12	8	28.50	17.69
-1	12	8	3.05	1.77
0	12	8	14.42	-11.70
1	12	8	3.05	-0.74
2	12	8	3.05	1.37
-3	12	9	3.05	1.44
-2	12	9	3.05	-2.65
0	12	9	3.05	1.06
-3	12	10	12.64	10.60
0	12	10	17.35	11.45
2	12	10	3.05	-2.95
1	13	0	3.05	-5.63
2	13	0	3.05	-8.86
3	13	0	9.85	-8.88
4	13	0	3.05	-4.76

Table 4 (*cont.*)

5	13	0	11.01	-10.60
6	13	0	3.05	5.79
-6	13	1	3.05	-0.02
-5	13	1	15.93	19.32
-4	13	1	13.60	14.90
-3	13	1	3.05	2.93
-2	13	1	12.79	-11.99
-1	13	1	13.35	-11.72
0	13	1	17.22	12.03
1	13	1	3.05	2.04
2	13	1	3.05	-1.03
3	13	1	10.00	7.98
4	13	1	3.05	4.44
5	13	1	9.49	-10.57
6	13	1	3.05	-4.87
-7	13	2	10.07	-7.96
-6	13	2	3.05	-1.02
-5	13	2	14.85	-15.26
-4	13	2	8.66	-9.41
-3	13	2	8.14	4.73
-2	13	2	3.05	1.13
-1	13	2	32.66	18.54
0	13	2	8.22	-0.36
1	13	2	7.00	-6.02
2	13	2	3.05	7.97
3	13	2	10.71	10.39
4	13	2	14.65	-13.29
5	13	2	3.05	-0.04
-6	13	3	8.72	8.44
-5	13	3	3.05	-3.53
-4	13	3	3.05	-4.05
-3	13	3	9.66	-10.29
-2	13	3	16.35	-11.86
-1	13	3	9.84	14.11
0	13	3	3.05	-7.45
1	13	3	7.53	-7.50
2	13	3	3.05	-2.14
3	13	3	3.05	-1.50
4	13	3	3.05	-3.20
-7	13	4	7.07	6.88
-6	13	4	3.05	-9.79
-5	13	4	3.05	-1.26
-4	13	4	18.32	5.94
-3	13	4	15.52	-17.51
-2	13	4	12.94	14.63
-1	13	4	11.87	13.91
0	13	4	9.72	11.99
1	13	4	3.05	3.31
2	13	4	3.05	7.37
3	13	4	3.05	0.53
-6	13	5	8.88	-8.97
-5	13	5	3.05	-6.89
-4	13	5	3.05	3.18
-3	13	5	3.05	-4.54
-2	13	5	17.94	15.35
-1	13	5	11.87	8.69
0	13	5	3.05	0.39
1	13	5	3.05	0.16
2	13	5	3.05	1.09
-5	13	5	3.05	1.61
-4	13	5	8.42	-12.08
-3	13	5	3.05	1.61
-2	13	5	20.61	-21.24
-1	13	5	3.05	-3.66
1	13	6	3.05	-2.07
2	13	6	3.05	0.67
-5	13	7	3.05	0.74
-4	13	7	6.89	-10.58
-3	13	7	3.05	3.04
-2	13	7	3.05	2.92
2	13	7	3.05	0.69
-5	13	8	3.05	-0.50
-4	13	8	14.37	17.10
-3	13	8	11.50	-7.66
-2	13	8	10.50	-5.37
2	13	8	3.05	2.80
-5	13	9	8.41	-5.40
-3	13	9	3.05	-0.77
-2	13	9	3.05	-4.64
0	14	0	3.05	-3.30
1	14	0	15.06	21.11
2	14	0	18.31	-24.37
3	14	0	3.05	1.50
4	14	0	18.64	32.04
5	14	0	7.85	-6.76
6	14	0	3.05	-3.02
-6	14	1	11.71	-7.30
-5	14	1	11.87	11.44
-4	14	1	3.05	-6.04
-3	14	1	13.97	15.76
-2	14	1	3.05	-6.29
-1	14	1	17.21	12.77
0	14	1	17.97	9.71
1	14	1	3.05	2.36
2	14	1	11.71	-7.16
3	14	1	3.05	-4.03
4	14	1	3.05	-1.31
5	14	1	21.08	20.80
6	14	1	3.05	-5.03
-7	14	2	21.52	-17.19
-6	14	2	3.05	-0.10
-5	14	2	30.86	32.45
-4	14	2	12.34	-11.47
-3	14	2	3.05	-0.88
-2	14	2	59.25	47.75
-1	14	2	3.05	3.10
0	14	2	8.59	-6.25
1	14	2	16.42	-10.44
2	14	2	3.05	2.77
3	14	2	9.84	-16.38
4	14	2	14.12	-18.40
5	14	2	3.05	0.62
-7	14	3	12.60	2.48
-6	14	3	12.78	12.33
-5	14	3	3.05	0.80
-4	14	3	10.60	14.16
-3	14	3	9.05	-7.73
-2	14	3	3.05	2.67
-1	14	3	45.52	-38.99
0	14	3	3.05	-5.49
1	14	3	3.05	-1.58
2	14	3	3.05	-4.18
3	14	3	3.05	0.63
4	14	3	4.73	-5.52
-6	14	4	3.05	2.58
-5	14	4	3.05	-4.72
-4	14	4	3.05	-3.89
-3	14	4	9.38	5.52
-2	14	4	18.53	30.14
-1	14	4	3.05	-5.43
0	14	4	29.60	-29.72
1	14	4	3.05	5.51
2	14	4	3.05	-1.59
3	14	4	12.09	-11.47
-6	14	5	7.50	-5.45
-5	14	5	3.05	-1.03
-4	14	5	7.94	3.47
-3	14	5	3.05	-2.88
-2	14	5	29.50	-36.06
-1	14	5	30.07	26.22
0	14	5	3.05	1.73
2	14	5	3.05	1.17
-5	14	6	3.05	-0.77
-4	14	6	5.67	5.83
-3	14	6	3.05	-6.62
-2	14	6	9.34	-8.66
-1	14	6	3.05	11.78
0	14	6	15.18	9.42
1	14	6	3.05	0.66
2	14	6	3.05	-5.74
-5	14	7	3.05	0.93
-4	14	7	7.02	-7.79
-3	14	7	3.05	-3.85
-2	14	7	33.52	31.93
-1	14	7	3.05	-1.98
0	14	7	3.05	0.72
2	14	7	3.05	0.64
-5	14	8	3.05	0.41
-4	14	8	28.32	-31.40
-3	14	8	11.62	-5.74
-2	14	8	3.05	3.17
-1	14	8	17.59	-14.90
2	14	8	12.20	9.57
-5	14	9	17.18	-8.43
-4	14	9	3.05	0.60
-3	14	9	3.05	7.09
-2	14	9	11.21	-6.36
-1	14	9	3.05	0.00
1	14	9	3.05	4.13
-4	14	10	13.05	9.98
1	15	0	7.01	10.59
2	15	0	25.97	31.44
3	15	0	3.05	2.20
4	15	0	3.05	9.75
5	15	0	17.04	16.91
6	15	0	3.05	-4.66
-6	15	1	3.05	1.03
-5	15	1	12.04	-13.99
-4	15	1	3.05	-2.71
-3	15	1	3.05	6.92
-2	15	1	11.68	12.75
-1	15	1	10.34	6.34
0	15	1	3.05	4.46
1	15	1	3.05	-3.79
2	15	1	12.01	-9.24
3	15	1	3.05	9.30
4	15	1	3.05	-9.18
5	15	1	3.05	2.33
6	15	1	3.05	2.49
-7	15	2	9.16	6.49
-6	15	2	3.05	3.71
-5	15	2	15.32	13.85
-4	15	2	15.59	17.96
-3	15	2	3.05	-0.71
-2	15	2	12.12	12.18
-1	15	2	3.05	0.35
0	15	2	23.23	-18.38
1	15	2	3.05	-0.33
2	15	2	3.05	-4.11
3	15	2	3.05	-3.38
4	15	2	3.05	4.53
5	15	2	3.05	0.60
-7	15	3	12.72	8.64
-6	15	3	3.05	-1.60
-4	15	3	3.05	3.18
-3	15	3	3.05	4.83
-2	15	3	3.05	2.41
0	15	3	9.74	10.90
-7	15	4	7.26	-6.19
-6	15	4	3.05	-3.41
-4	15	4	3.05	0.93
-3	15	4	14.44	-10.91
-2	15	4	16.01	-23.01
0	15	4	3.05	-3.25
-6	15	5	7.54	4.92
-4	15	5	3.05	3.97
-3	15	5	15.13	10.87
-2	15	5	3.05	-33.02
-4	15	6	6.87	8.84
-3	15	6	3.05	9.24
-2	15	6	20.75	23.68
-4	15	7	6.09	6.20
-3	15	7	16.77	-13.30
-2	15	7	3.05	0.05
-4	15	8	11.79	-12.48
-3	15	8	3.05	1.32
-2	15	8	10.66	10.00
0	16	0	93.85	89.40
1	16	0	3.05	[illegible]
2	16	0	26.74	-32.63
3	16	0	20.04	13.42
4	16	[illegible]	[illegible]	[illegible]
5	16	0	14.69	-27.13
-7	16	1	12.49	-6.32
-5	16	1	16.44	21.61
-4	16	1	3.05	-2.43
-3	16	1	3.05	-0.76
-2	16	1	3.05	2.03
-1	16	1	3.05	-8.16
0	16	1	3.05	-5.27
1	16	1	23.28	-18.05
2	16	1	3.05	-5.41
3	16	1	3.05	-3.83
4	16	1	14.61	-14.07
5	16	1	3.05	2.01
-6	16	2	16.38	11.56
-5	16	2	3.05	2.89
-4	16	2	22.72	-27.12
-3	16	2	15.03	16.50
-2	16	2	3.05	-0.64
-1	16	2	3.05	-1.18
0	16	2	24.23	-23.63
1	16	2	3.05	-2.38
2	16	2	25.74	25.23
3	16	2	3.05	-3.14
4	16	2	3.05	-2.87
5	16	2	12.32	11.85
-7	16	3	11.41	7.36
-5	16	3	12.53	-14.66
-4	16	3	3.05	-2.80
-3	16	3	3.05	-3.39
-2	16	3	19.17	17.21
-1	16	3	3.05	1.03
0	16	3	14.28	-15.62
1	16	3	8.31	-5.50
5	16	3	3.05	-1.92
-4	16	4	19.41	14.39
-3	16	4	15.00	-8.38
-2	16	4	8.82	12.98
-1	16	4	13.21	-19.20
0	16	4	3.05	-0.92
1	16	4	13.64	9.30
-8	16	5	11.39	9.75
-6	16	5	7.70	-7.60
-4	16	5	3.05	0.95
-3	16	5	3.05	0.26
-2	16	5	20.15	-22.45
-1	16	5	3.05	-2.45
0	16	5	11.00	7.49
-4	16	6	11.24	23.78
-3	16	6	3.05	-3.83
-2	16	6	52.65	-55.72
-1	16	6	15.88	17.20
0	16	6	3.05	2.09
1	16	6	25.41	-21.51
-4	16	7	9.39	-11.61
-3	16	7	11.50	-6.42
-2	16	7	3.05	2.42
-1	16	7	3.05	-0.87
-4	16	8	3.05	-5.50
-3	16	8	3.05	5.96
-2	16	8	29.46	26.27
-4	16	9	8.00	12.82
1	17	0	11.70	11.52
2	17	0	27.82	-36.57
3	17	0	11.40	-9.78
4	17	0	14.42	-9.54
5	17	0	8.00	-14.64
-5	17	1	14.30	15.72
-4	17	1	3.05	-1.75
-3	17	1	13.60	-14.05
-2	17	1	3.05	7.84
-1	17	1	3.05	1.50
0	17	1	3.05	-6.20
1	17	1	3.05	6.59
2	17	1	3.05	4.91
3	17	1	3.05	-5.88
4	17	1	3.05	3.68
5	17	1	3.05	-3.70
-4	17	2	28.37	-35.22
-3	17	2	10.90	-13.11
-2	17	2	3.05	-1.85
-1	17	2	3.05	-1.97
0	17	2	16.24	15.59
1	17	2	3.05	-3.88
2	17	2	3.05	9.89
3	17	2	3.05	0.71
4	17	2	3.05	-5.57
-7	17	3	11.46	-7.04
-4	17	3	3.05	3.56
-3	17	3	3.05	0.44
-2	17	3	3.05	3.06
-1	17	3	3.05	7.28
0	17	3	10.42	-12.55
1	17	3	3.05	2.35
-7	17	4	7.38	1.20
-4	17	4	6.52	6.18
-3	17	4	17.36	13.59
-2	17	4	9.09	8.81
-1	17	4	3.05	9.60
0	17	4	3.05	0.55
1	17	4	13.91	7.73
-6	17	5	7.91	-4.90
-4	17	5	3.05	-1.50
-3	17	5	3.05	-2.86
-2	17	5	16.26	18.65
-1	17	5	3.05	-6.64
-4	17	6	7.18	13.00
-3	17	6	3.05	-0.91
-2	17	6	21.63	-14.84
-1	17	6	24.41	-24.42
1	17	6	3.05	1.56
-4	17	7	11.75	-15.20
-3	17	7	3.05	3.43
-2	17	7	3.05	5.00
-1	17	7	3.05	-1.76
-4	17	8	6.56	9.48
-2	17	8	3.05	-4.78
0	18	0	3.05	2.99
1	18	0	12.19	-12.62
2	18	0	28.89	-37.74
3	18	0	3.05	0.92
4	18	0	44.85	53.08
5	18	0	3.05	-8.46
-5	18	1	3.05	6.12
-4	18	1	3.05	0.16
-3	18	1	9.20	-5.34
-2	18	1	3.05	3.10
-1	18	1	11.80	9.62
0	18	1	12.94	-11.02
1	18	1	3.05	4.42
2	18	1	3.05	2.13
3	18	1	22.02	-15.22
4	18	1	3.05	-0.55
5	18	1	10.21	7.74
-5	18	2	24.30	20.96
-4	18	2	29.20	-32.92
-3	18	2	3.05	4.86
-2	18	2	24.15	21.84
-1	18	2	3.05	-1.28
0	18	2	16.88	-15.43
1	18	2	3.05	2.36
2	18	2	3.05	3.59
3	18	2	3.05	1.32
4	18	2	15.69	-11.99
5	18	2	3.05	0.31
-7	18	3	11.49	5.86
-6	18	3	11.06	5.43
-5	18	3	3.05	0.41
-4	18	3	3.05	0.06
-3	18	3	3.05	-3.23
-2	18	3	3.05	-2.34
-1	18	3	20.20	-15.04
0	18	3	3.05	-7.42
1	18	3	3.05	-1.68
3	18	3	3.05	-0.64
-5	18	4	6.64	-11.00
-4	18	4	3.05	-0.86
-3	18	4	17.79	-19.65
-2	18	4	21.34	20.27
-1	18	4	3.05	-2.79
0	18	4	3.05	0.37
1	18	4	14.17	8.42
3	18	4	12.91	-8.12
-6	18	5	8.07	-4.71
-4	18	5	7.52	9.61
-2	18	5	16.67	-15.34
-1	18	5	3.05	3.98
0	18	5	3.05	3.06
-4	18	6	3.05	5.86
-2	18	6	3.05	-5.63
-1	18	6	30.10	28.74
0	18	6	11.65	10.97
1	18	6	3.05	-1.20
-4	18	7	9.62	-12.82
-2	18	7	22.43	19.43
-1	18	7	3.05	-3.30
0	18	7	3.05	-5.61
-4	18	8	11.61	-12.13
-2	18	8	3.05	0.84
-1	18	8	34.68	-26.98
0	19	0	3.05	0.86
2	19	0	26.39	27.82
3	19	0	3.05	-4.31
4	19	0	3.05	7.18
5	19	0	3.05	6.96
-5	19	1	3.05	-3.85
-4	19	1	3.05	-1.17
-3	19	1	3.05	4.05
-2	19	1	3.05	-5.60
-1	19	1	3.05	4.71
0	19	1	3.05	4.23
1	19	1	12.89	-11.24
2	19	1	3.05	3.92
3	19	1	9.91	6.03
4	19	1	3.05	-3.20
5	19	1	3.05	-1.41
-5	19	2	7.70	8.48
-4	19	2	24.78	29.28
-3	19	2	3.05	-1.38
-2	19	2	3.05	2.85
-1	19	2	3.05	3.84
0	19	2	27.10	-21.19
1	19	2	3.05	-2.70
2	19	2	3.05	-8.93
3	19	2	3.05	4.53
4	19	2	3.05	2.04
5	19	2	3.05	2.12
-4	19	3	3.05	-0.05
-3	19	3	3.05	-5.85
-2	19	3	6.87	-6.16
-1	19	3	3.05	2.20
0	19	3	3.05	5.12
1	19	3	3.05	3.06
2	19	3	3.05	1.30
-4	19	4	3.05	-9.12
-3	19	4	16.47	-11.70
-2	19	4	14.10	-14.41
-1	19	4	3.05	-6.08
1	19	4	16.82	-15.36
3	19	4	3.05	1.67
-4	19	5	3.05	0.61
-3	19	5	3.05	6.98
-2	19	5	10.00	-6.16
-1	19	5	3.05	-0.08
3	19	5	3.05	-0.74
-4	19	6	3.05	-6.38
-3	19	6	3.05	2.22
-2	19	6	3.05	8.71
-1	19	6	30.34	23.79
1	19	6	3.05	-0.59
3	19	6	3.05	-3.92
-4	19	7	7.67	8.47
-3	19	7	3.05	-2.57
-2	19	7	3.05	-0.90
-1	19	7	3.05	1.73
3	19	7	3.05	0.98
-4	19	8	3.05	1.56
-2	19	8	11.47	8.85
0	20	0	27.17	27.84
1	20	0	3.05	0.80
2	20	0	23.03	-22.69
3	20	0	15.10	-6.50
-3	20	1	3.05	-0.34
-2	20	1	17.30	14.57
-1	20	1	3.05	-4.02
0	20	1	3.05	-3.23
1	20	1	3.05	-2.43
2	20	1	3.05	3.88
3	20	1	3.05	1.39
-6	20	2	10.20	7.41
-4	20	2	18.02	-24.36
-3	20	2	3.05	-0.88
-2	20	2	3.05	2.01
-1	20	2	3.05	0.11
0	20	2	27.97	-22.00
1	20	2	3.05	1.41
2	20	2	34.27	34.84
3	20	2	3.05	2.47
5	20	2	11.07	8.02
-5	20	3	9.07	-8.47
-3	20	3	3.05	10.95
-2	20	3	6.99	-7.02
-1	20	3	3.05	0.86
0	20	3	3.05	-1.31
1	20	3	3.05	4.32
2	20	3	3.05	1.94
3	20	3	3.05	-1.26
-3	20	4	3.05	-4.12
-2	20	4	6.36	7.33
-1	20	4	29.34	-26.24
0	20	4	3.05	1.20
1	20	4	22.30	20.00
2	20	4	3.05	-1.33
3	20	4	3.05	-1.18
-3	20	5	19.15	-11.16
-2	20	5	3.05	-2.05
-1	20	5	3.05	-0.42
0	20	5	11.63	10.58
-2	20	6	17.60	-19.55
-1	20	6	25.00	20.21
0	20	6	3.05	-0.20
1	20	6	14.93	-13.33
-2	20	7	3.05	1.08
-1	20	7	3.05	4.56
-2	20	8	11.62	17.97
-4	20	9	12.27	9.33
1	21	0	3.05	-2.30
2	21	0	18.54	-18.35
3	21	0	3.05	-0.81
4	21	0	3.05	-2.02
-4	21	1	3.05	-1.21
-3	21	1	9.94	-9.76
-2	21	1	3.05	5.57
-1	21	1	3.05	0.80
0	21	1	3.05	-1.25
1	21	1	3.05	0.43
2	21	1	14.60	-12.95
3	21	1	3.05	3.24
4	21	1	3.05	1.80
-4	21	2	17.03	-14.49
-3	21	2	3.05	-1.25
-2	21	2	3.05	0.85
-1	21	2	3.05	3.66
0	21	2	11.09	11.28
1	21	2	3.05	-9.56
2	21	2	3.05	2.32
3	21	2	3.05	-5.32
4	21	2	3.05	-3.83
-3	21	3	10.87	14.19
-2	21	3	3.05	1.63
-1	21	3	3.05	-5.52
0	21	3	3.05	6.14
1	21	3	3.05	-7.02
2	21	3	3.05	5.38
3	21	3	3.05	0.59
-2	21	4	3.05	3.69
-1	21	4	3.05	0.86
1	21	4	18.18	18.05
2	21	4	3.05	4.51
-1	21	5	3.05	4.12
1	21	5	3.05	4.99
-1	21	6	17.98	-17.23
1	21	6	3.05	-0.15
0	22	0	3.05	3.52
1	22	0	3.05	5.17
2	22	0	18.93	-17.71
3	22	0	3.05	0.89
4	22	0	27.36	23.44
-4	22	1	3.05	2.94
-3	22	1	22.09	-22.33
-2	22	1	3.05	3.27
-1	22	1	3.05	3.76
0	22	1	14.78	-10.87
1	22	1	3.05	-0.28
2	22	1	16.25	16.49
3	22	1	3.05	-1.29
4	22	1	3.05	0.32
5	22	1	10.44	-7.59
-4	22	2	3.05	-11.34
-3	22	2	3.05	-0.15
-2	22	2	3.05	6.32
-1	22	2	3.05	5.13
0	22	2	3.05	-6.32
1	22	2	32.68	-31.30
2	22	2	3.05	1.29
3	22	2	9.10	8.90
4	22	2	3.05	-8.22
-4	22	3	3.05	-9.31
-3	22	3	13.91	14.59
-2	22	3	3.05	-0.34
-1	22	3	3.05	0.71
0	22	3	3.05	8.89
1	22	3	3.05	7.84
2	22	3	3.05	-8.64
3	22	3	3.05	0.33
-5	22	4	18.79	-13.41
-4	22	4	3.05	0.58
-1	22	4	3.05	0.44
0	22	4	11.65	13.14
1	22	4	14.23	12.35
-4	22	5	12.44	13.20
-2	22	5	3.05	-2.74
-1	22	5	3.05	3.00
0	22	5	3.05	-0.29
1	22	5	14.84	-12.62
2	22	5	3.08	-3.42
-1	22	6	15.66	13.33
1	22	6	3.05	-0.84
1	23	0	3.05	4.58
2	23	0	12.67	9.57
3	23	0	3.05	-0.63
4	23	0	3.05	0.44
-4	23	1	3.05	-1.02
-3	23	1	3.05	-1.01
-2	23	1	3.05	-8.81
-1	23	1	3.05	4.32
1	23	1	3.05	-3.98
2	23	1	14.96	11.62
3	23	1	3.05	-3.15
4	23	1	3.05	3.80
-4	23	2	3.05	6.82
-3	23	2	3.05	0.15
-2	23	2	3.05	-3.23
-1	23	2	8.52	-9.82
1	23	2	3.05	5.15
2	23	2	3.05	-4.17
3	23	2	3.05	6.91
4	23	2	3.05	6.86
-4	23	3	8.23	-3.76
-3	23	3	11.17	-12.36
-2	23	3	3.05	2.53
-1	23	3	3.08	-1.69
1	23	3	12.33	12.92
2	23	3	3.05	0.86
3	23	3	3.08	-0.79
-2	23	4	3.05	3.89
-1	23	4	3.05	-0.93
1	23	4	12.86	-10.33
2	23	4	3.08	-7.57
-1	23	5	3.05	-0.68
-1	23	6	8.83	8.53
0	24	0	3.05	-2.38
1	24	0	3.05	2.79
2	24	0	3.05	-4.81
3	24	0	16.38	-5.87
-3	24	1	3.05	-0.39
-2	24	1	15.31	13.86
-1	24	1	3.05	5.32
0	24	1	3.05	1.79
1	24	1	3.05	1.32
2	24	1	3.05	8.19
3	24	1	3.05	4.97
-3	24	2	3.05	-6.74
-2	24	2	3.05	0.30
-1	24	2	12.22	13.89
0	24	2	3.05	0.76
1	24	2	3.05	0.22
2	24	2	25.86	21.01
3	24	2	3.05	3.95
-3	24	3	14.53	13.91
-2	24	3	10.37	-15.74
-1	24	3	3.08	-1.24
0	24	3	11.75	5.73
1	24	3	12.72	9.44
2	24	3	3.05	0.65
3	24	3	13.52	-11.66
-3	24	4	3.05	6.84
-2	24	4	3.05	-3.63
-1	24	4	31.25	-36.24
1	24	4	13.12	11.70
2	24	4	17.24	-14.43
-3	24	5	15.06	-16.88
-2	24	5	10.95	11.06
-1	24	5	3.05	1.91
-3	24	6	21.29	1.06
1	25	0	14.40	-11.95
2	25	0	3.05	0.22
3	25	0	3.05	2.78
-3	25	1	3.05	1.20
-2	25	1	3.05	3.33
-1	25	1	3.05	-2.24
1	25	1	3.05	-2.77
2	25	1	15.78	-9.94
3	25	1	3.05	4.61
-3	25	2	3.05	3.84
-2	25	2	3.05	0.82
-1	25	2	3.05	8.49
1	25	2	3.05	-3.11
2	25	2	3.05	-0.19
-3	25	3	14.96	12.59
-2	25	3	3.05	1.45
-1	25	3	3.05	-2.99
1	25	3	3.05	-4.22
3	25	3	3.05	-0.81
-2	25	4	3.05	1.04
-1	25	4	3.05	0.43
1	25	4	13.31	10.44
-2	25	5	11.19	-10.10
2	25	6	3.05	-0.32
1	26	0	14.92	11.74
0	26	1	31.19	-22.05
1	26	2	36.23	-26.22
-3	26	3	15.30	13.46
-3	26	4	21.33	12.30
-3	27	4	19.32	7.53

ture factor $\frac{1}{2} F_{min} = 3{\cdot}00$. The value 3·05 given in Table 4 for unobserved reflexions is a result of change of scale factor in the course of the refinement. The weak $\bar{1}11$ reflexion was omitted, as it was not possible to measure it with certainty owing to the disturbing effect of white radiation in both orientations.

All calculations were performed on a National Elliott 803B computer, with programs developed in our laboratory. The Fourier syntheses were calculated by means of programs using matrix operations according to Jaggi (1960). The least-squares program used in this work is the same as formerly applied by Toman & Očená-šková (1964).

The resulting fractional coordinates and isotropic individual temperature coefficients, together with their standard deviations, are given in Table 3. A survey of the observed and calculated structure factors is given in Table 4.

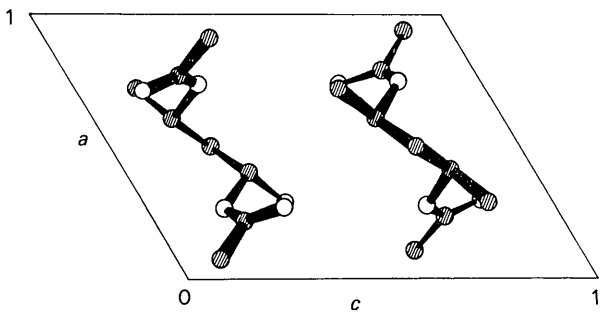

Fig. 3. Projection of the structure between planes $y = -0{\cdot}1$ and $y = +0{\cdot}1$ along the unique b axis. Molecules are related through a centre of symmetry at (0·5, 0, 0·5).

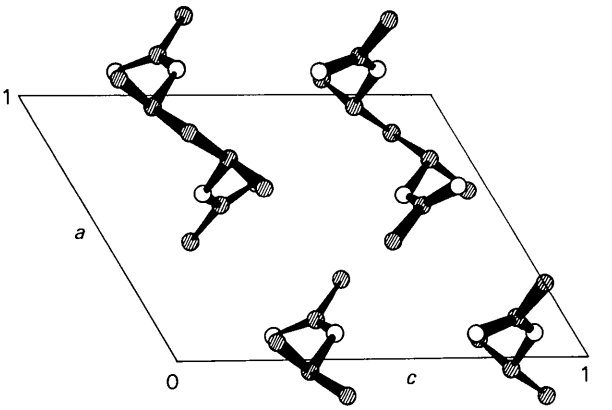

Fig. 4. Projection of the structure between planes $y = 0{\cdot}15$ and $y = 0{\cdot}35$ along the unique b axis. Molecules are related through a glide plane (x, 0·25, z).

Table 5. *Interatomic intramolecular vectors and angles*

Molecule at $y=0$		Molecule at $y=0{\cdot}25$		Standard value*
C(1)–C(2)	1·54 Å	C(10)–C(11)	1·53 Å	1·54 Å
C(2)–C(3)	1·53	C(11)–C(12)	1·52	
C(3)–C(4)	1·51	C(12)–C(13)	1·53	
C(4)–C(5)	1·51	C(13)–C(14)	1·52	
C(2)–O(1)	1·49	C(11)–O(5)	1·46	1·47
C(4)–O(2)	1·46	C(13)–O(6)	1·47	
O(1)–C(6)	1·32	O(5)—C(15)	1·34	1·36
O(2)–C(7)	1·32	O(6)—C(16)	1·31	
C(6)–O(3)	1·23	C(15)–O(7)	1·22	1·23
C(7)–O(4)	1·25	C(16)–O(8)	1·28	
C(6)–C(8)	1·50	C(15)–C(17)	1·50	1·52
C(7)–C(9)	1·52	C(16)–C(18)	1·51	
O(3)–O(4)	4·95	O(7)—O(8)	4·89	
O(3)–C(9)	4·95	O(7)—C(18)	4·88	
C(8)–O(4)	4·93	C(17)–O(8)	4·94	
C(8)–C(9)	5·94	C(17)–C(18)	5·95	
C(1)–C(2)–C(3)	116°	C(10)–C(11)–C(12)	112°	
C(2)–C(3)–C(4)	116	C(11)–C(12)–C(13)	113	
C(3)–C(4)–C(5)	114	C(12)–C(13)–C(14)	110	
C(1)–C(3)–C(5)	179	C(10)–C(12)–C(14)	177	
C(1)–C(2)–O(1)	106	C(10)–C(11)–O(5)	109	
C(3)–C(2)–O(1)	105	C(12)–C(11)–O(5)	106	
C(5)–C(4)–O(2)	107	C(14)–C(13)–O(6)	107	
C(3)–C(4)–O(2)	105	C(12)–C(13)–O(6)	107	
C(2)–O(1)–C(6)	117	C(11)–O(5)—C(15)	118	
C(4)–O(2)–C(7)	117	C(13)–O(6)—C(16)	121	
O(1)–C(6)–O(3)	123	O(5)—C(15)–O(7)	121	
O(2)–C(7)–O(4)	123	O(6)—C(16)–O(8)	118	
O(1)–C(6)–C(8)	114	O(5)—C(15)–C(17)	113	
O(2)–C(7)–C(9)	114	O(6)—C(16)–C(18)	117	
O(3)–C(6)–C(8)	123	O(7)—C(15)–C(17)	126	
O(4)–C(7)–C(9)	123	O(8)—C(16)–C(18)	125	

* According to *International Tables for X-Ray Crystallography* (1962).

Conformation of the molecule

Two independent left-handed molecules have the same geometry within the limits of the standard deviations of interatomic vectors and angles, which are listed in Table 5. The final conformation of the left-handed molecule is given in Fig. 6. The e.s.d. for atomic positions of carbon and oxygen atoms, derived from standard deviations of fractional coordinates from least-squares refinement, is 0·02 Å, for interatomic vectors 0·03 Å and for intervector angles about 3·5°. O(1)–C(6), O(2)–C(7), O(5)–C(15) and O(6)–C(16) bonds, which have a mean value of 1·32 Å, are significantly shorter than O(1)–C(2), O(2)–C(4), O(5)–C(12) and O(6)–C(14), which have the mean value 1·47 Å as a result of conjugation of the carbonyl oxygen atoms O(3), O(4), O(7) and O(8).

The geometry of the molecule, which represents the most interesting feature of the structure, was analysed by calculating equations of the best planes passing through the atoms of acetate groups and those of the pentane chain, according to Schomaker, Waser, Marsh & Bergman (1959). The best planes were determined with the same weight assigned to all atoms. Normals of these planes, interplanar angles and displacements of atomic positions from the best planes are summarized in Table 6.

Root-mean-square displacement of atoms from the plane calculated for the atoms of the pentane chain is greater than the e.s.d. for atomic positions, and therefore the pentane chain seems to be slightly twisted along C(2)–C(3) and C(3)–C(4) bonds.

The interplanar angles between the triangle through atoms C(1)–C(2)–C(3) and that through C(3)–C(4)–C(5) are 10·5° and 7·5° for the molecules at $y=0$ and $y=\frac{1}{4}$ respectively. Non-planarity of the pentane chain can be easily seen from the *h*0*l* projections (Figs. 3 and 4).

The acetate groups of the molecule of pentane-2,4-diol diacetate are planar, and the interesting feature of

Table 6. *Plane – normal vector summary*

$xm_1+ym_2+zm_3-d=0$ x, y, z – monoclinic fractional coordinates

Plane	Atoms comprising the plane	Displacements (Å)	R.M.S. displacement (Å)	m_1	m_2	m_3	d(Å)
I	C(1)	−0·0292	0·0414	+3·2084	+0·0543	+6·6613	+3·2737
	C(2)	+0·0587					
	C(3)	−0·0008					
	C(4)	−0·0582					
	C(5)	+0·0295					
II	C(10)	−0·0087	0·0352	+3·2507	+0·6611	+6·6077	+8·5832
	C(11)	+0·0454					
	C(12)	−0·0301					
	C(13)	−0·0428					
	C(14)	+0·0361					
III	C(2)	−0·0138	0·0223	+7·2599	+13·0061	−5·2294	+0·9366
	C(6)	+0·0414					
	C(8)	−0·0225					
	O(1)	+0·0062					
	O(3)	−0·0108					
IV	C(4)	+0·0072	0·0163	+7·5856	−10·6772	−5·7098	+3·7194
	C(7)	−0·0314					
	C(9)	+0·0139					
	O(2)	+0·0008					
	O(4)	+0·0096					
V	C(11)	−0·0004	0·0007	+7·5807	+10·6586	−5·8585	+0·2861
	C(15)	+0·0012					
	C(17)	−0·0006					
	O(5)	+0·0002					
	O(7)	−0·0004					
VI	C(13)	−0·0161	0·0143	+7·2730	−12·9289	−5·1962	−0·0001
	C(16)	+0·0153					
	C(18)	−0·0156					
	O(6)	+0·0169					
	O(8)	−0·0004					

Interplanar angles

I –III = 70·8°	II–V = 71·4°
I –IV = 71·5	II–VI = 71·0
III–IV = 51·0	V–VI = 50·9

Table 7(*a*). *Intermolecular intralayer contacts less than* 4·5 Å

Layer at $y=0$					Layer at $y=0{\cdot}25$				
From atom	in molecule	to atom	in molecule	d(Å)	From atom	in molecule	to atom	in molecule	d(Å)
O(3)	*L*1	O(4)	*L*3	4·07	O(7)	*L*4	O(8)	*L*6	4·10
O(3)	*L*1	C(9)	*L*3	3·45	O(7)	*L*4	C(18)	*L*6	3·48
C(8)	*L*1	O(4)	*L*3	3·40	C(17)	*L*4	O(8)	*L*6	3·47
C(8)	*L*1	C(9)	*L*3	4·22	C(17)	*L*4	C(18)	*L*6	4·31
C(1)	*L*1	C(5)	*L*3	3·99	C(10)	*L*4	C(14)	*L*6	4·09
O(3)	*L*1	C(1)	*D*2	3·50	O(8)	*L*4	C(10)	*D*5	3·45
O(3)	*L*1	C(2)	*D*2	3·51	O(8)	*L*4	C(11)	*D*5	3·59
O(3)	*L*1	C(3)	*D*2	3·98	O(8)	*L*4	C(12)	*D*5	3·92
C(9)	*L*1	C(1)	*D*2	3·82	C(17)	*L*4	C(10)	*D*5	3·85

Table 7(*b*). *Intermolecular interlayer contacts less than* 4·5 Å

Between layer at $y=0$ and layer at $y=0{\cdot}25$					Between layer at $y=0{\cdot}25$ and layer at $y=0{\cdot}50$				
From atom	in molecule	to atom	in molecule	d(Å)	From atom	in molecule	to atom	in molecule	d(Å)
C(9)	*L*1	C(17)	*D*5	4·12	C(17)	*L*4	C(8)	*D*7	3·88
C(9)	*L*1	O(7)	*D*5	3·71	C(17)	*L*4	O(3)	*D*7	4·16
C(9)	*L*1	C(18)	*D*5	3·91	C(17)	*L*4	C(9)	*D*7	4·13
C(9)	*L*1	O(8)	*D*5	4·16	C(17)	*L*4	O(4)	*D*7	3·75
O(4)	*L*1	C(17)	*D*5	3·74	O(7)	*L*4	C(9)	*D*7	3·72
C(8)	*L*1	C(17)	*D*5	3·88	C(18)	*L*4	C(9)	*D*7	3·94
O(3)	*L*1	C(17)	*D*5	4·16	O(8)	*L*4	C(9)	*D*7	4·17
C(8)	*L*1	O(8)	*D*8	3·68	C(18)	*L*4	O(3)	*D*9	3·67
O(3)	*L*1	C(18)	*D*8	3·70	O(8)	*L*4	C(8)	*D*9	3·68
O(3)	*L*1	O(8)	*D*8	3·95	O(8)	*L*4	O(3)	*D*9	3·95
C(1)	*D*2	C(12)	*L*4	4·22	C(10)	*D*5	C(3)	*L*10	4·35
C(3)	*D*2	C(10)	*L*4	4·35	C(12)	*D*5	C(1)	*L*10	4·22
C(5)	*D*2	C(14)	*L*6	3·98	C(14)	*D*5	C(5)	L11	3·98

Molecules in Tables 7(*a*) and 7(*b*).

Molecule	
*L*1	Atoms C(1), C(2), · · · , O(4)
*D*2	Molecule *L*1 at $1-x;\ -y;\ 1-z$
*L*3	*L*1 at $x-1;\ y;\ z$
*L*4	Atoms C(10), C(11), · · · , O(8)
*D*5	Molecule *L*4 at $x\ ;\ 0{\cdot}5-y;\ -0{\cdot}5+z$
*L*6	*L*4 at $x-1;\ y\ ;\ z$
*D*7	*D*2 at $1-x;\ 0{\cdot}5+y;\ 1{\cdot}5-z$
*D*8	*D*5 at $x-1;\ y\ ;\ z$
*D*9	*D*7 at $x+1;\ y\ ;\ z$
*L*10	*L*1 at $1-x;\ 0{\cdot}5+y;\ 0{\cdot}5-z$
*L*11	*L*10 at $x+1;\ y\ ;\ z$

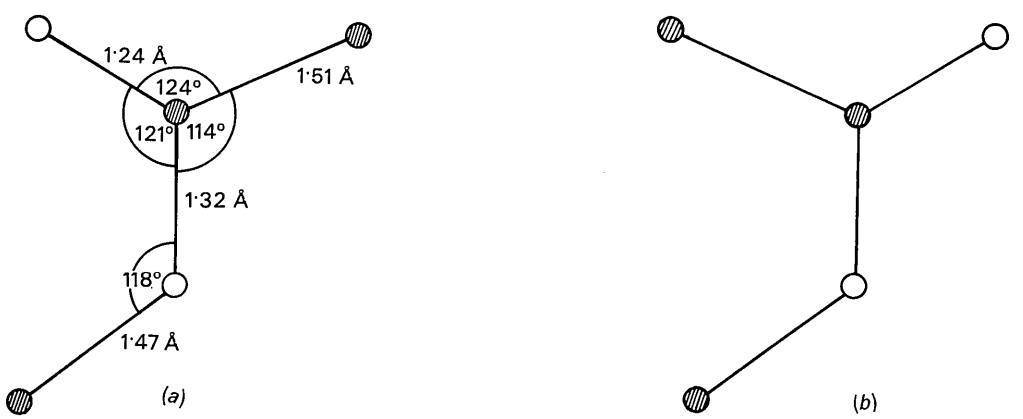

Fig. 5. Two possible conformations of the acetate group in the molecule of pentane-2,4-diol diacetate. The resultant conformation of the acetate group as found from output coordinates is given in (*a*).

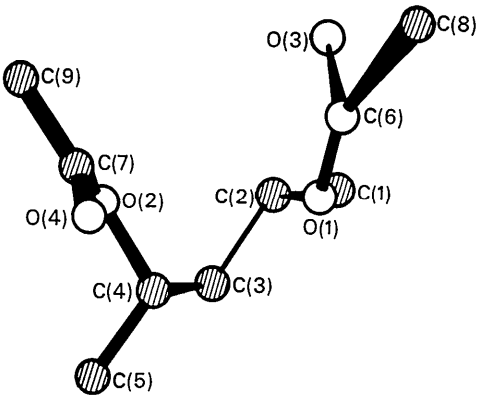

Fig. 6. Resultant conformation and numbering of atoms of the first independent left-handed molecule of pentane-2,4-diol diacetate at $y=0$. In the second independent molecule atoms C(10), C(11), ..., O(8) correspond to C(1), C(2),....., O(4) atoms respectively.

the geometry of molecule is that they are not coplanar, as one could expect; their interplanar angle is 51°; the interatomic distance between neighbouring carbonyl oxygen atoms O(3)–O(4) and O(7)–O(8) is about 4·9 Å – a distance much larger than that corresponding to van der Waals atomic radii. The cause of this is not quite clear; it could perhaps be explained by coulombic repulsion of equally charged carbonyl oxygen atoms or by steric influence of the methyl group of a neighbouring molecule.

Packing

Eight molecules are placed in a unit cell in four layers. In spite of the fact that molecules in different layers are coupled by different elements of symmetry (centre of symmetry and glide plane), the inner structure of both layers is the same within the limits of the standard deviations. Intermolecular contacts shorter than 4·5 Å are given in Table 7. An overall view of the structure of pentane-2,4-diol diacetate showing the packing of the molecules is in Fig. 7.

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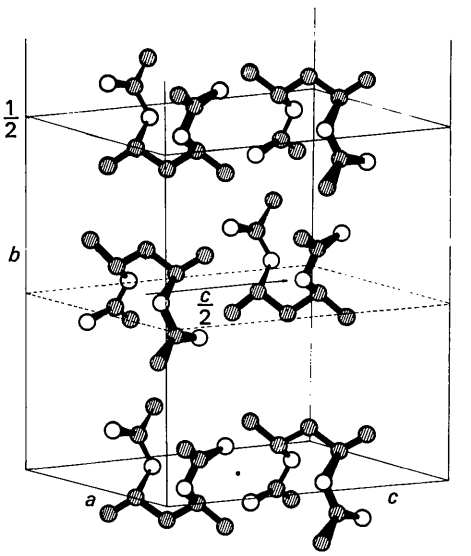

Fig. 7. Overall view of the crystal structure of the DL form of pentane-2,4-diol diacetate.

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