In the refinements of the 250 and 268°C data, the occupancy of the alternate oxygen sites was a free parameter, and at 268°C it seems clear that there is partial occupancy of these sites. Above the 275°C transition, to refine the 290°C data we assumed equal occupancy of the '*e*' sites and the alternative sites and allocated the two sets of oxygen atoms separate positions and thermal parameters. The low *R* value, and the agreement between the two sets of oxygen position parameters, support this hypothesis of the structure.

The mean square vibration amplitude of Na, N and O atoms, calculated as $\frac{1}{3}(u_{11}+u_{22}+u_{33})$, is plotted against temperature in Fig. 1, together with the results of CHP. The spectacular increase in the O vibrations, reported by CHP, seems to be spurious. The 268° data gave anomalously low values for the vibration amplitudes and we suspect that this was caused by fairly intense diffuse scattering resulting in anomalous absorption.

If the NO_3 group is rigid, then u_{11} for N and O should be the same. Table 1 shows that this is indeed so, within the quoted error limits, up to 250°C. The rotational amplitude of the NO_3 group about the *c* axis (the 3-axis of our Cartesian system) is not unusually large (11·7° at 250°C).

The bond length from the conventional refinements decreases with temperature due to the well-known apparent shortening due to arc motion. Refinements incorporating a proper formulation of this effect gave a more-or-less constant value of the N–O distance at 1·256 (1) Å. The agreement with CHP on this point is excellent.

Analysis of X-ray data

Taking the thermal and positional parameters at room temperature from this experiment, and the X-ray data of Inkinen and CHP (put on a common scale by separate refinements), we prepared difference Fouriers.

The X-ray form factors of $Na^+N^{2+}O_3^-$ and of $Na^+N^{5+}O_3^{2-}$ were calculated after Clementi (1965). These difference Fouriers appeared, however, to show no systematic features which could be interpreted as clear information on the ionic state or bonding within the NO_3 group. We concluded that more accurate X-ray data would be needed to explore this question.

References

Cherin, P., Hamilton, W. C. & Post, B. (1967). *Acta Cryst.* **23**, 455.

Clementi, E. (1965). *IBM J. Res. Dev.* **9**, 2, plus Supplementary Tables of Atomic Functions.

Inkinen, O. (1960). *Ann. Acad. Sci. Fenn., Series A*, **55**, 1.

International Tables for X-ray Crystallography (1965). Vol. I. Birmingham: Kynoch Press.

Pryor, A. W., Ellis, P. J. & Dullow, R. J. (1968). *J. Appl. Cryst.* **1**, 272.

Pryor, A. W. & Sanger, P. L. (1970). *Acta Cryst.* A**26**, 543.

Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558.

Acta Cryst. (1972). B**28**, 2702

The Crystal Structure of *p*-Nitrophenyl Acetate

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The crystal structure of *p*-nitrophenyl acetate, $C_8H_7NO_4$, is monoclinic, $P2_1/c$, $a=14{\cdot}115$ (10), $b=7{\cdot}437$ (9), $c=16{\cdot}158$ (10) Å, $\beta=90{\cdot}83$ (5)°, $Z=8$, $T=23$°C, $D_x=1{\cdot}42$ g.cm^{-3}, $D_m=1{\cdot}37$ g.cm^{-3}. The intensities of 2234 independent reflexions were measured with a four-circle diffractometer. The structure was solved using the symbolic addition method and refined by full-matrix least-squares analysis to a weighted least-squares residue of 0·048. In both of the two independent molecules, the plane of the acyl group is rotated approximately 65° from the plane of the phenyl ring and both molecules have the *trans* conformation. The C–NO_2 bond lengths are similar to those in related compounds with electron donating substituents.

Introduction

p-Nitrophenyl acetate has been used extensively in studies of alkaline hydrolysis and enzyme catalysed hydrolysis (see *e.g.* Boyer, Lardy & Myrback, 1960) because of the ease of estimation of nitrophenol by spectrophotometry and the relative simplicity of the molecule. Simple steric arguments suggest that either the acyl group must be rotated from the plane of the phenyl ring or the molecule must adopt the *cis* conformation rather than the more stable *trans* conformation. This study was undertaken to determine the conformation of the molecule and provide information on the bonding scheme in the acyl linkage.

Experimental

Samples were prepared from *p*-nitrophenol by Chattaway's method (Chattaway, 1931) and recrystallized from ethanol. A sample of approximate dimensions $0{\cdot}2 \times 0{\cdot}2 \times 0{\cdot}5$ mm was selected for data collection and aligned on a Picker card-fed diffractometer. The Laue symmetry and systematic extinctions gave the space group $P2_1/c$.

The integrated intensities of the 2234 independent reflexions between 0 and 45° in 2θ were collected with Mo $K\alpha$ radiation using a graphite monochromator. The θ–2θ scan mode was used with a scan rate of 2·0° min^{-1} over a base width of 2·4°. The background on each side was counted for 10 sec.

In order to obtain accurate lattice constants, 31 reflexions with good intensities and 2θ values between 37 and 45° were chosen from the collected data. A second crystal was mounted on the diffractometer and the 31 reflexions were centred. The least-squares values of the lattice constants were calculated with the program *PICK*2, written by W. C. Hamilton. The estimated errors given in brackets with the lattice constants are three times the estimated standard deviations determined from the least-squares analysis. Comparison of lattice constants determined from separate sets of reflexions from one crystal and from separate crystals suggest that this is a reasonable estimate of real error.

Crystal data

$a = 14{\cdot}115$ (10) Å	Space group $P2_1/c$
$b = 7{\cdot}437$ (9)	$V = 1696$ Å^3
$c = 16{\cdot}158$ (10)	F.W. 181·15
$\beta = 90{\cdot}83$ (5)°	$Z = 8$
$\mu(\text{Mo } K\alpha) = 1{\cdot}25 \text{ cm}^{-1}$	$D_m = 1{\cdot}37 \text{ g.cm}^{-3}$ (flotation)
$\lambda(\text{Mo } K\alpha)_1 = 0{\cdot}70926$	$D_x = 1{\cdot}42 \text{ g.cm}^{-3}$
$T = 23\,^\circ\text{C}$	$F(000) = 752$.

The data were corrected for Lorentz and polarization effects but no absorption corrections were applied. A Wilson statistical calculation was used to normalize the data to the contents of one unit cell and to obtain an overall temperature factor of 3.75 Å^2. Individual reflexions were labelled as weak if both $\text{Lp}|F_o| < 7{\cdot}0$ and $|F_o| < 2\sigma$ obtained. The estimated standard deviation, σ, used here is calculated as $\sigma' + 0{\cdot}5 + 0{\cdot}005|F_o|$ where σ' is calculated from the counting statistics of the integrated intensity and the background counts. The number of reflexions which survived as reliable data was 1396. The remaining data were not used for the structure solution or the initial stages of refinement but were retained and used in the final cycles of least-squares refinement. The standard deviation of each weak reflexion was replaced by $|F_o|$ for that reflexion or 10·0, whichever was greater. The scattering factors of the carbon, oxygen and nitrogen atoms were calculated from the series coefficients given by Cromer & Mann (1968). Those for the hydrogen atoms were calculated from the coefficients given by Moore (1963) weighted for optimum accuracy at low scattering angles.

Determination and refinement of the structure

The 411 reflexions with $|E| > 1{\cdot}30$ were selected and used in the multiple-solution, logical symbolic addition method programs of Germain & Woolfson (1968). An E map calculated from the solution with the highest figure of merit showed all the non-hydrogen atoms of both molecules in the asymmetric unit.

The positions and isotropic temperature factors of these atoms were refined by full-matrix least-squares analysis using a modified version of the program *ORFLS* (Busing, Martin & Levy, 1962). Only 720 reliable reflexions with 2θ values between 11 and 37° were used at this point. After eight cycles of least squares, an R_w value of 0·121 was reached and anisotropic temperature factors were introduced. The agreement index R_w used here is calculated as

$$R_w = [\sum w(|F_o| - |F_c|)^2 / \sum w|F_o|^2]^{1/2} \text{ with } w = \sigma^{-2}.$$

Because of computer core size limitation, the two molecules were then refined separately on alternate cycles for a total of four cycles, reducing the R_w value to 0·084. A difference Fourier map calculated at this point revealed eight of the 14 hydrogen atoms and another map after four more cycles of least-squares gave the locations of the remaining six hydrogen atoms. The isotropic temperature factors of the phenyl hydrogen atoms were set at 5·0 Å^2 and those of the methyl group were set at 7·0 Å^2. All the data were used in the final 14 cycles of least squares. The estimated standard deviations, σ, used in the σ^{-2} weighting scheme, of the reliable reflexions were replaced by the series

$$\sigma = 2{\cdot}028 - 0{\cdot}926|F_o| + 0{\cdot}00134|F_o|^2.$$

These coefficients were determined by fitting to a curve of $\Delta = ||F_o| - |F_c||$ plotted against $\langle |F_o| \rangle$. The method assumes that F_c is nearer to the true structure factor than F_o and thus $\langle \Delta \rangle$ is a reasonable estimate for σ. The weak reflexions were not included in the calculation of the coefficients for σ and the original estimated standard deviations were used in the refinement because the large uncertainties in these reflexions require higher order terms in the expression for σ. The final R_w value for all data was 0·049 and for the reliable data alone the final R_w value was 0·048. The conventional R value for reliable data was 0·082, and 0·165 if all the data was included. The standard deviations of the least-square variables were slightly lower when the large body of weak data were included in the refinement. An unusually large number of reflexions appear to be below the background count rate, reflecting the large magnification of truncation errors associated with short background count times. This systematic error may occur despite the fact that one-half dekacount is added to each observed number of counts, if

Table 1. *Observed and calculated structure factors for p-nitrophenyl acetate* (× 10)

The reflexions marked with an asterisk were considered as being weak.

		|FO|	FC
H	L	K = 0	
0	2	109	114
0	4	241	236
0	6	214	-210
0	8	211	-213
0	10	348	352
0	12	76	71
0	14	392	394
0	16	112	119
1	-16	136	138
1	-14	46	114
1	-12	53	-67
1	-10	81	-65
1	-8	84	-80
1	-6	90	-118
1	-4	388	384
1	-2	80	83
1	0	83	-24
1	2	497	-487
1	4	421	-419
1	6	573	-555
1	8	614	606
1	10	122	131
1	12*	15	-37
1	14*	33	-32
1	16	196	-203
2	-16*	18	-25
2	-14*	40	-45
2	-12*	9	-38
2	-10	90	-125
2	-8	169	-156
2	-6	215	230
2	-4	575	590
2	-2	463	460
2	0	659	678
2	2	183	176
2	4	1061	1045
2	6	472	-477
2	8	750	713
2	10*	31	-28
2	12	148	-140
2	14	215	213
2	16*	0	55
3	-16	90	-70
3	-14*	0	101
3	-12	56	42
3	-10	48	22
3	-8	37	49
3	-6	1126	1163
3	-4	319	308
3	-2	966	-1019
3	0*	0	-17
3	2	1685	-1377
3	4	551	561
3	6	132	129
3	8	441	437
3	10*	0	-6
3	12	61	-67
3	14	125	-118
3	16	93	-92
4	-16	78	85
4	-14	88	-93
4	-12	115	-103
4	-10	149	146
4	-8*	18	-20
4	-6	248	-234
4	-4	322	-330
4	-2	601	-611
4	0	508	508
4	2	348	372
4	4	223	-221
4	6	107	-96
4	8	408	-396
4	10	268	-262
4	12	56	88
4	14*	0	38
4	16	65	100
5	-16	119	-115
5	-14	58	62
5	-12*	34	-27
5	-10	97	95
5	-8*	0	0
5	-6*	0	11
5	-4	265	-265
5	-2	228	220
5	0	99	85
5	2	680	669
5	4	268	297
5	6	1134	-1057
5	8	326	321
5	10*	37	54
5	12*	0	63
5	14	118	157
5	16*	19	-19
6	-16*	0	-10
6	-14	140	138
6	-12	75	48
6	-10	295	-296
6	-8	262	-245
6	-6	272	-272
6	-4	161	138
6	-2	742	730
6	0	1013	1019
6	2	528	-536
6	4	57	-60
6	6	328	-325
6	8	225	-218
6	10*	22	38
6	12	112	113
6	14	173	184
6	16*	35	6
7	-14	57	-48
7	-12*	0	50
7	-10	50	-46
7	-8	213	-213
7	-6*	0	-48
7	-4	400	406
7	-2	167	-189
7	0	86	-80
7	2	242	-248
7	4	364	-355
7	6	433	425
7	8	98	123
7	10*	29	65
7	12	86	98
7	14	91	-88
8	-14	162	160
8	-12	154	-124
8	-10	125	131
8	-8	142	-137
8	-6	70	85
8	-4	293	288
8	-2	98	64
8	0	536	510
8	2*	16	-57
8	4	253	245
8	6	127	-131
8	8	338	337
8	10*	0	-8
8	12	68	-84
8	14*	43	88
9	-14*	43	22
9	-12*	0	-31
9	-10*	37	-116
9	-8	388	393
9	-6	303	301
9	-4	327	-335
9	-2	246	-233
9	0*	36	-43
9	2	208	-212
9	4	301	294
9	6	120	-114
9	8	310	316
9	10	59	56
9	12	145	-166
9	14*	49	-17
10	-12	61	-14
10	-10*	0	59
10	-8*	0	-129
10	-6	58	-78
10	-4	130	-133
10	-2	101	-118
10	0	315	309
10	2*	0	53
10	4*	0	-18
10	6	176	-160
10	8	172	-173
10	10	53	-50
10	12	67	74
11	-12*	29	8
11	-10*	0	15
11	-8	164	-140
11	-6*	0	30
11	-4	125	119
11	-2	72	78
11	0*	0	40
11	2*	0	9
11	4	199	-198
11	6	281	-281
11	8	336	336
11	10	114	-90
11	12	66	80
12	-10	222	-206
12	-8	109	-115
12	-6	188	-183
12	-4*	40	-76
12	-2*	0	1
12	0	137	-131
12	2*	0	-124
12	4*	23	-113
12	6	233	-241
12	8	101	-113
12	10*	29	-8
13	-8	76	-105
13	-6	199	192
13	-4*	9	-14
13	-2	78	71
13	0	66	-67
13	2*	0	10
13	4*	34	-6
13	6	109	-98
13	8*	21	61
14	-6*	0	-30
14	-4*	14	-16
14	-2	197	-186
14	0	149	-143
14	2	102	119
14	4	61	-80
14	6*	33	-12
15	-4*	19	-14
15	-2*	0	-11
15	0	51	-30
15	2*	0	-10
H	L	K = 1	
0	0*	10	0
0	1	204	-201
0	2	119	-130
0	3	293	289
0	4	30	-8
0	5	253	-247
0	6	172	159
0	7	298	-294
0	8	115	110
0	9*	28	45
0	10	186	-195
0	11*	13	31
0	12	344	344
0	13	48	55
0	14	58	68
0	15	125	-148
0	16	146	-165
0	17	89	90
1	-16*	0	16
1	-15	81	-109
1	-14*	32	-36
1	-13*	17	-26
1	-12*	0	7
1	-11	70	-68
1	-10	181	183
1	-9*	0	7
1	-8	345	347
1	-7	105	102
1	-6	177	192
1	-5	57	60
1	-4*	23	21
1	-3	290	289
1	-2	835	895
1	-1	384	-395
1	0	26	22
1	1	33	-64
1	2	834	878
1	3	626	-641
1	4	285	281
1	5	73	87
1	6	276	-273
1	7	228	-217
1	8	163	164
1	9	71	65
1	10	109	111
1	11	166	172
1	12	97	103
1	13*	0	9
1	14	64	73
1	15	47	63
1	16	87	93
1	17	89	-77
2	-16*	28	54
2	-15	69	-61
2	-14*	0	23
2	-13	78	-74
2	-12	143	160
2	-11*	0	-19
2	-10	173	-171
2	-9	159	-152
2	-8	449	-449
2	-7*	0	-43
2	-6	122	-128
2	-5	269	274
2	-4	773	-819
2	-3	687	738
2	-2	1130	1251
2	-1*	0	-12
2	0	789	823
2	1	863	-896
2	2	1008	-1083
2	3	442	447
2	4	161	-157
2	5	31	-38
2	6	338	-356
2	7*	29	7
2	8	74	44
2	9	189	-192
2	10	136	125
2	11*	21	16
2	12*	0	20
2	13	170	184
2	14	66	62
2	15	62	-59
2	16*	0	-29
2	17*	10	32
3	-16	149	152
3	-15	116	-108
3	-14*	0	-3
3	-13*	0	69
3	-12*	38	46
3	-11	110	-119
3	-10*	0	7
3	-9	369	377
3	-8	347	342
3	-7	369	-361
3	-6	387	398
3	-5*	21	-12
3	-4	787	851
3	-3	262	258
3	-2	961	961
3	-1	135	-154
3	0	46	3
3	1	204	213
3	2	314	319
3	3	522	-529
3	4	624	-615
3	5	712	699
3	6	929	913
3	7*	26	-20
3	8	518	489
3	9*	0	-20
3	10*	0	34
3	11	71	-74
3	12	198	196
3	13*	20	41
3	14	69	-69
3	15*	0	1
3	16	72	-50
4	-16*	37	103
4	-15*	0	-22
4	-14	102	112
4	-13*	0	12
4	-12	65	-66
4	-11	60	34
4	-10*	31	-18
4	-9*	26	43
4	-8	123	135
4	-7*	0	-11
4	-6	229	-212
4	-5	310	-324
4	-4	398	404
4	-3	68	-50
4	-2	136	-159
4	-1	269	272
4	0	838	-839
4	1	657	657
4	2	398	391
4	3	127	133
4	4	51	-63
4	5	133	153
4	6	198	178
4	7	87	-100
4	8*	29	47
4	9	38	45
4	10*	28	-57
4	11	42	-57
4	12	93	-69
4	13	56	-42
4	14*	35	-35
4	15*	0	8
4	16	65	-60
5	-16*	0	30
5	-15	66	78
5	-14	49	19
5	-13*	0	-2
5	-12*	0	-40
5	-11	41	17
5	-10	188	-197
5	-9	172	188
5	-8	374	371
5	-7	73	-70
5	-6	558	546
5	-5	116	-135
5	-4	83	-86
5	-3	408	-415
5	-2	191	-188
5	-1	386	397
5	0	146	136
5	1	60	55
5	2	434	-443
5	3*	0	64
5	4	156	164
5	5	35	28
5	6	224	209
5	7*	0	14
5	8*	0	-18
5	9	49	68
5	10	215	200
5	11*	0	-20
5	12	78	-81
5	13	45	19
5	14*	13	33
5	15*	0	-57
6	-16*	18	66
6	-15*	0	-26
6	-14	115	-117
6	-13	110	122
6	-12*	0	41
6	-11	150	-159
6	-10*	38	85
6	-9*	0	38
6	-8	107	116
6	-7	118	-122
6	-6*	0	-12
6	-5	265	256
6	-4	45	-48
6	-3	214	213
6	-2	104	-97
6	-1	213	-210
6	0	165	170
6	1	61	66
6	2	98	-92
6	3	129	-125
6	4	96	83
6	5	53	40
6	6	231	229
6	7	120	-116
6	8	216	-226
6	9	166	168
6	10	44	-14
6	11*	0	-38
6	12	53	20
6	13*	32	44
6	14*	0	-13
6	15*	0	-47
7	-15*	0	-30
7	-14*	0	9
7	-13*	0	-5
7	-12*	33	-48
7	-11*	20	30
7	-10	145	158
7	-9*	0	4
7	-8*	19	54
7	-7	79	82
7	-6	201	-199
7	-5	167	167
7	-4	205	202
7	-3	93	83
7	-2	79	88
7	-1	212	-214
7	0	134	123
7	1	289	-290
7	2	160	142
7	3	189	-196
7	4	291	-296
7	5	94	106
7	6	156	-148
7	7	75	83
7	8	221	213
7	9*	37	-7
7	10*	0	-50
7	11*	0	21
7	12*	0	58
7	13*	0	4
7	14	113	120
7	15*	0	-18
8	-14	52	46
8	-13	67	-46
8	-12*	0	-31
8	-11*	0	-33
8	-10	169	-164
8	-9	50	-29
8	-8	101	-105
8	-7	60	34
8	-6*	35	-33
8	-5	90	85
8	-4*	23	-51
8	-3	69	-65
8	-2	319	322
8	-1	71	-70
8	0*	0	33
8	1	166	-176
8	2	274	-279
8	3	118	112
8	4	83	83
8	5	100	-99
8	6	90	-80
8	7	66	-39
8	8	101	123
8	9*	40	-22
8	10	96	51
8	11*	0	-7
8	12*	33	12
8	13*	0	20
8	14	61	18
9	-14*	0	6
9	-13*	21	5
9	-12	63	63
9	-11*	23	-55
9	-10	53	60
9	-9	147	152
9	-8	208	215
9	-7	150	-167
9	-6	290	291
9	-5*	0	-28
9	-4	113	114
9	-3*	15	-56
9	-2	152	168
9	-1	112	-122
9	0	147	137
9	1	141	148
9	2*	0	-55
9	3*	17	13
9	4	179	176
9	5	168	177
9	6	396	397
9	7	253	-247
9	8	48	28
9	9	80	-29
9	10	88	85
9	11*	0	11
9	12	74	76
9	13*	0	5
10	-13*	0	11
10	-12*	0	-40
10	-11*	20	19
10	-10*	0	-16
10	-9	124	-125
10	-8	118	-124
10	-7	48	-30
10	-6	51	59
10	-5	160	-164
10	-4*	0	0
10	-3	119	121
10	-2	54	-39
10	-1	44	47
10	0	106	-117
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9	-5*	0	-22
9	-4*	0	-22
9	-3*	16	21
9	-2*	0	7
9	-1*	48	-58
9	0	59	37
9	1	92	85
9	2	51	55
9	3	77	-74
9	4	87	103
9	5*	0	-9
10	-2*	25	20
10	-1	56	-10
10	0	66	81
10	1*	0	-52
10	2	38	46
H	L	K = 7	
0	0	49	0
0	1*	31	29
0	2	218	223
0	3*	0	37
0	4*	0	21
0	5	85	-75
0	6	93	112
0	7	51	-33
0	8	93	-84
1	-8*	0	-19
1	-7*	0	-24
1	-6	56	-73
1	-5	58	-36
1	-4	105	-133
1	-3	79	15
1	-2	113	106
1	-1*	0	27
1	0	49	56
1	1*	20	-58
1	2	86	95
1	3*	40	25
1	4*	33	58
1	5*	0	13
1	6	113	-129
1	7*	47	40
1	8*	0	-3
2	-8*	0	20
2	-7	90	-90
2	-6*	0	8
2	-5*	0	-18
2	-4*	47	-37
2	-3*	0	-8
2	-2	130	116
2	-1	63	-55
2	0	144	157
2	1	62	49
2	2*	0	-10
2	3*	20	16
2	4*	0	3
2	5*	0	13
2	6*	0	6
2	7*	49	-66
2	8*	0	19
3	-8	63	-32
3	-7	140	120
3	-6*	0	-34
3	-5*	28	-15
3	-4	113	125
3	-3*	0	42
3	-2*	3	-7
3	-1	56	-64
3	0*	39	28
3	1*	0	-29
3	2*	0	-63
3	3	63	68
3	4	118	-123
3	5*	0	-13
3	6	87	70
3	7*	33	64
3	8	75	-25
4	-7*	43	-55
4	-6*	42	67
4	-5*	14	53
4	-4*	46	36
4	-3*	31	25
4	-2*	28	-11
4	-1*	0	-8
4	0	133	-146
4	1*	0	-25
4	2*	18	60
4	3*	44	29
4	4*	0	25
4	5*	0	-2
4	6*	0	16
4	7	93	-113
5	-6*	24	-19
5	-5*	21	12
5	-4	103	-116
5	-3	149	151
5	-2	157	-150
5	-1*	41	-2
5	0*	44	-31
5	1*	0	-23
5	2	75	-39
5	3*	0	-19
5	4	74	98
5	5*	0	-1
5	6	64	-33
6	-5*	0	-30
6	-4	88	-112
6	-3	74	76
6	-2	91	-113
6	-1	74	58
6	0	97	90
6	1*	0	44
6	2*	0	30
6	3*	38	-42
6	4*	0	-17
6	5*	10	-6
7	-3*	36	91
7	-2*	9	1
7	-1	74	32
7	0	61	-77
7	1	91	-79
7	2*	0	18
7	3*	0	25
H	L	K = 8	
0	0	90	-69
0	1*	0	-9
0	2*	0	25
1	-2*	0	-8
1	-1*	0	-24
1	0*	0	-4
1	1*	0	46
1	2*	0	-57
2	-1*	0	22
2	0	125	133
2	1*	0	-8

Table 2. *Positional and thermal parameters*

The U_{ij} are given in Å^2 and are multiplied by 10^3. The temperature-factor expression is $\exp\,[-2\pi^2(U_{11}a^{*2}h^2+\ldots 2U_{12}a^*b^*hk\ldots)]$. The numbers in parentheses are estimated errors.

	x/a	y/b	z/c	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	0·3925 (9)	0·1176 (17)	0·7097 (8)	49 (9)	42 (9)	58 (9)	1 (6)	9 (6)	−3 (6)
C(2)	0·3452 (10)	0·2037 (20)	0·6457 (9)	43 (9)	73 (12)	66 (9)	10 (9)	3 (9)	13 (9)
C(3)	0·3933 (10)	0·2533 (21)	0·5766 (9)	54 (9)	84 (12)	58 (9)	6 (9)	3 (9)	20 (9)
C(4)	0·4872 (9)	0·2140 (17)	0·5715 (8)	42 (9)	53 (9)	51 (9)	−2 (9)	3 (6)	−3 (6)
C(5)	0·5342 (11)	0·1277 (21)	0·6361 (10)	50 (12)	76 (12)	87 (12)	18 (9)	1 (9)	−6 (6)
C(6)	0·4870 (11)	0·0807 (19)	0·7042 (10)	60 (12)	57 (9)	69 (9)	8 (9)	−5 (9)	13 (6)
C(7)	0·2392 (15)	0·0694 (29)	0·8880 (11)	92 (12)	77 (15)	52 (9)	−4 (12)	3 (9)	14 (12)
C(8)	0·2973 (9)	0·1698 (24)	0·8262 (8)	45 (9)	65 (9)	39 (9)	1 (12)	−9 (6)	−10 (9)
N	0·5377 (9)	0·2640 (16)	0·4972 (8)	62 (9)	60 (9)	77 (9)	−11 (12)	11 (9)	−5 (9)
O(1)	0·6218 (7)	0·2348 (16)	0·4937 (6)	58 (6)	139 (12)	110 (9)	5 (12)	29 (6)	18 (9)
O(2)	0·4926 (7)	0·3325 (16)	0·4391 (6)	88 (9)	115 (9)	61 (6)	−10 (6)	2 (6)	13 (6)
O(3)	0·3447 (6)	0·0516 (12)	0·7778 (6)	72 (6)	48 (6)	60 (6)	1 (6)	3 (6)	4 (6)
O(4)	0·3036 (6)	0·3291 (14)	0·8200 (6)	75 (6)	48 (6)	68 (6)	−4 (6)	−2 (6)	−5 (6)
C(1′)	0·8807 (8)	0·1720 (17)	0·4920 (8)	47 (9)	33 (6)	56 (9)	−1 (6)	4 (6)	−4 (6)
C(2′)	0·9675 (9)	0·2510 (17)	0·5002 (9)	56 (9)	56 (9)	52 (9)	−12 (9)	16 (6)	17 (9)
C(3′)	1·0191 (9)	0·2384 (18)	0·5737 (8)	49 (9)	50 (9)	56 (9)	−1 (9)	−7 (6)	3 (9)
C(4′)	0·9807 (8)	0·1433 (18)	0·6366 (7)	44 (9)	55 (9)	39 (9)	3 (6)	−1 (6)	7 (6)
C(5′)	0·8935 (9)	0·0616 (20)	0·6295 (9)	48 (9)	66 (9)	56 (9)	−4 (9)	10 (9)	13 (6)
C(6′)	0·8422 (9)	0·0759 (18)	0·5558 (8)	43 (9)	47 (9)	63 (9)	−10 (9)	−1 (6)	−3 (6)
C(7′)	0·7381 (19)	0·3117 (37)	0·3123 (12)	93 (15)	92 (18)	51 (12)	−10 (15)	−21 (12)	1 (12)
C(8′)	0·7960 (8)	0·3339 (22)	0·3896 (8)	48 (9)	53 (9)	48 (9)	−3 (9)	10 (6)	−2 (9)
N′	1·0331 (10)	0·1319 (17)	0·7153 (8)	73 (9)	79 (9)	59 (9)	−10 (9)	−6 (9)	15 (6)
O(1′)	0·9929 (8)	0·0719 (18)	0·7743 (7)	119 (9)	189 (15)	59 (9)	−53 (9)	−23 (6)	41 (6)
O(2′)	1·1148 (7)	0·1820 (16)	0·7164 (5)	61 (6)	132 (9)	92 (9)	−12 (9)	−20 (6)	3 (6)
O(3′)	0·8304 (6)	0·1732 (12)	0·4165 (5)	81 (6)	45 (6)	51 (6)	4 (6)	−21 (6)	−6 (6)
O(4′)	0·8070 (6)	0·4696 (12)	0·4268 (5)	63 (6)	46 (6)	64 (6)	−1 (6)	−9 (6)	0 (6)

Table 2 (*cont.*)

	x/a	y/b	z/c	B
H(2)	0·276 (10)	0·235 (17)	0·655 (7)	5·0
H(3)	0·364 (9)	0·317 (19)	0·530 (8)	5·0
H(5)	0·596 (10)	0·110 (19)	0·626 (8)	5·0
H(6)	0·519 (9)	0·019 (19)	0·752 (9)	5·0
H(7,1)	0·270 (11)	−0·025 (24)	0·908 (10)	7·0
H(7,2)	0·217 (10)	0·153 (25)	0·938 (9)	7·0
H(7,3)	0·181 (11)	0·019 (23)	0·860 (9)	7·0
H(2′)	0·996 (9)	0·310 (18)	0·453 (7)	5·0
H(3′)	1·083 (9)	0·292 (19)	0·581 (8)	5·0
H(5′)	0·867 (9)	0·004 (19)	0·672 (8)	5·0
H(6′)	0·781 (9)	0·009 (18)	0·549 (7)	5·0
H(7′,1)	0·765 (14)	0·253 (26)	0·286 (12)	7·0
H(7′,2)	0·729 (11)	0·433 (23)	0·282 (10)	7·0
H(7′,3)	0·672 (12)	0·277 (21)	0·330 (8)	7·0

the number of individual counts for each background measurement averages near a multiple of ten.

Results and discussion

The observed and calculated structure factors of all reflexions are given in Table 1. The final positional and thermal parameters are given in Table 2. The estimated errors given here are three times the estimated standard deviations calculated from the diagonal components of the inverse least-squares matrix.

The atoms making up the two molecules are numbered with the same sequence and those belonging to the second molecule are marked with a prime. The relevant interatomic distances and angles are given in Fig. 1 with the labelling sequence of the atoms. The estimated errors in the bond lengths are based only on the errors given in Table 2. Inclusion of the errors associated with the lattice constants would increase these values by *ca.* 0·001 Å. Both molecules have the *trans* configuration but the plane of the acyl group is rotated from that of the phenyl ring by 64·2 and 65·9° in the first and second molecule. The parameters describing the least-squares planes fitted to the nitro groups, the acyl groups and the phenyl rings are given in Table 3 with the dihedral angles between these planes.

The bonds N–O(1), N–O(2), C(8)–O(4) and C(8)–C(7) are terminal bonds and are affected by thermal motion. Table 4 shows corrections to these bond lengths made on the assumption that they undergo 'riding motion', as suggested by Busing & Levy (1964). The thermal corrections bring the (N–O) bonds within the accepted limits for NO_2^- groups. The C=O bond lengths correspond to those of carbonyl bonds in conjugated systems and the methyl bond is slightly shortened from the expected single-bond value. The proper model for the basis of thermal corrections to the O(3)–C(8) bond is not clear, but a 'riding motion' correction gives 1·366 and 1·373 Å for the first and second molecules respectively.

These bond lengths indicate the presence of some delocalization in the acyl group. This delocalization inhibits the double-bonded character of the bond from the O(3) atom to the phenyl ring with the result that the C(1)–O(3) bond lengths of 1·388 and 1·402 Å in the two molecules of *p*-nitrophenyl acetate are markedly longer than the phenyl carbon to oxygen bond

Table 3. *Least-squares planes*

Coordinates refer to the directions of the *a,b,c** axes

Plane				
1.	$-0·2126x-0·8843y-0·4157z$	=	−6·6835	(Aromatic ring, molecule 1)
2.	$-0·7619x-0·0037y-0·6476z$	=	−11·7054	(Acyl group, molecule 1)
3.	$-0·1834x-0·9100y-0·3716z$	=	−6·1471	(Nitro group, molecule 1)
4.	$0·4415x-0·8323y-0·3351z$	=	1·7114	(Aromatic ring, molecule 2)
5.	$0·8315x+0·1641y-0·5307z$	=	6·3106	(Acyl group, molecule 2)
6.	$0·3014x-0·9209y-0·2473z$	=	0·5832	(Nitro group,molecule 2)

Table 3 (*cont.*)

Perpendicular distances. (Atoms defining the plane have their distances marked with an asterisk.)

	Plane 1	Plane 2	Plane 3
C(1)	−0·0014*	−0·1824	−0·1017
C(2)	−0·0033*		−0·0230
C(3)	0·0062*		0·0254
C(4)	−0·0044*	−0·5827	−0·0270
C(5)	−0·0004*		−0·1041
C(6)	0·0033*		−0·1383
C(7)		0·0017*	
C(8)		−0·0061*	
N	−0·0190		0·0000*
O(1)	0·0182		0·0000*
O(2)	−0·0912		0·0000*
O(3)	−0·1246	0·0019*	
O(4)		0·0025*	
H(2)	0·0576		
H(3)	0·0227		
H(5)	−0·0004		
H(6)	0·0103		

	Plane 4	Plane 5	Plane 6
C(1′)	0·0027*	0·0796	0·0149
C(2′)	−0·0041*		0·2200
C(3′)	0·0026*		0·2134
C(4′)	0·0003*	0·2093	−0·0186
C(5′)	−0·0017*		−0·2365
C(6′)	0·0002*		−0·2197
C(7′)		0·0066*	
C(8′)		−0·0228*	
N′	0·0371		0·0000*
O(1′)	0·2419		0·0000*
O(2′)	−0·1559		0·0000*
O(3′)	−0·0925	0·0070*	
O(4′)		0·0092*	
H(2′)	−0·0773		
H(3′)	−0·0262		
H(5′)	0·0422		
H(6′)	−0·0706		

Dihedral angles

Planes 1 and 2	64·2°
Planes 1 and 3	3·3
Planes 4 and 5	65·9
Planes 4 and 6	10·8

lengths of 1·352 Å in the *β* modification of *p*-nitrophenol (Coppens & Schmidt, 1965*a*) and 1·350 Å in anisic acid (Bryan, 1967).

Table 5 compares some pertinent features of simple aromatic molecules containing NO_2 groups in the *para* position. The double-bonded contribution to the C–NO_2 bond tends to increase as the electron donating character of the *para* substituent becomes greater. The angle between the plane of the NO_2 group and the plane of the ring does not appear to be related to the electron donating character of the *para* substituent and is perhaps more dependent on steric effects.

Mak & Trotter (1965) have discussed the shortening of the central C–C bonds in the phenyl rings caused by contributions from the quinonoid valence structure which also tends to increase the double-bonded character of the C–NO_2 bond. The lengths of the central C–C bonds are also given in Table 5.

Packing diagrams in two projections are shown in Figs. 2 and 3. All intermolecular contacts involving non-hydrogen atoms less than 3·4 Å in length are shown in addition to all contacts involving hydrogen atoms less than 2·8 Å in length. The first molecule is involved in a total of 32 such contacts and the second in 28. These seem to be rather large numbers of contacts in comparison with the equivalent numbers for the compounds in Table 5. The 2·36 Å contact between the carbonyl oxygen atom of the second molecule and the H(3) atom of another second molecule, related to the first by a 2_1 operator is shorter than the sum of the van der Waals radii of the two atoms. Coppens & Schmidt (1965*b*) have reported an aromatic hydrogen atom in the structure of the *α* modification of *p*-nitrophenol to be within 2·38 Å of an oxygen atom belonging to the nitro substituent on another molecule.

Most of the small differences between the two independent molecules are of no chemical interest and are presumably caused by the packing of the structure. The difference between the average central C–C bond lengths in the two molecules is large but is nevertheless slightly less than the sum of the combined errors in the two sets of bond lengths. Further, there is no significant difference in the environment of the two molecules which might account for a variation in the bonding. The average of all four central C–C bond lengths is 1·376 Å which is in good agreement with the other central C–C bonds in Table 5 for compounds with short C–NO_2 bonds.

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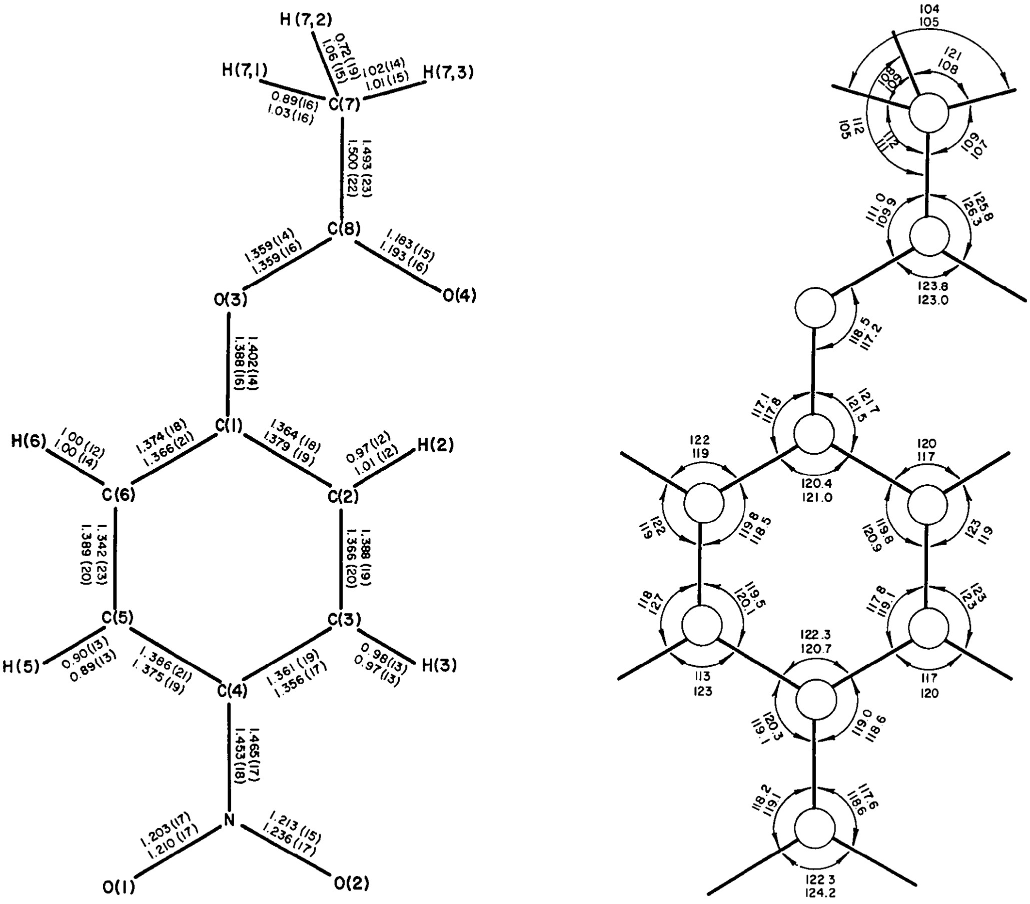
Table 4. *Terminal bond lengths corrected for thermal motion*

	Bond lengths (Å)			
	First molecule		Second molecule	
	Uncorrected	Corrected	Uncorrected	Corrected
N–O(1)	1·210	1·257	1·203	1·264
N–O(2)	1·236	1·267	1·213	1·246
C(8)–O(4)	1·193	1·218	1·183	1·194
C(8)–C(7)	1·500	1·525	1·493	1·526

Table 5. *Comparison of p-nitrophenyl acetate with related compounds*

	Angle between plane of NO_2 group and phenyl plane	Average length of central C–C bonds	C–NO_2 bond length
p-Nitroaniline (Trueblood, Goldish & Donohue, 1961)	1·9°	1·375 Å	1·460 Å
p-Nitrophenol (Coppens & Schmidt, 1965)	7·9	1·375	1·460
N,*N*-Dimethyl-*p*-nitroaniline (Mak & Trotter, 1965)	3	1·37	1·40
p-Nitrophenyl acetate (molecule 1)	3·3	1·354	1·454
p-Nitrophenyl acetate (molecule 2)	10·8	1·388	1·465
p-Nitrotoluene (Barve & Pant, 1971)	3·0	1·382	1·482
p-Nitrobenzoic acid (Tavale & Pant, 1971)	13·8	1·382	1·485
p-Nitroperoxybenzoic acid (Kim, Chu & Jeffrey, 1970)	6	1·43	1·52



(*a*) (*b*)

Fig. 1. (*a*) Schematic representation of the molecule with bond lengths and labelling sequence. The number nearest the line is the bond length of the first molecule. (*b*) Bond angles. The number nearest the atom is the bond angle of the first molecule.

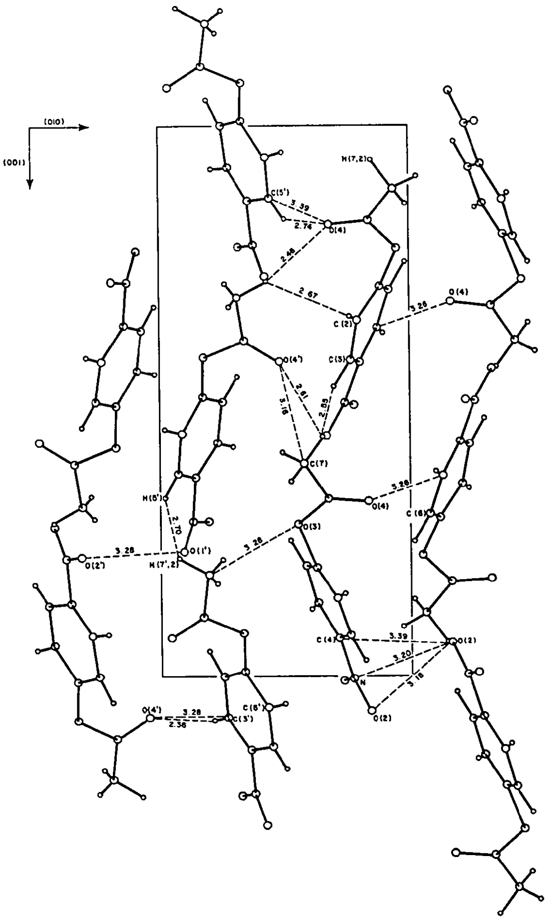


Fig. 2. Packing diagram in the [001] projection.

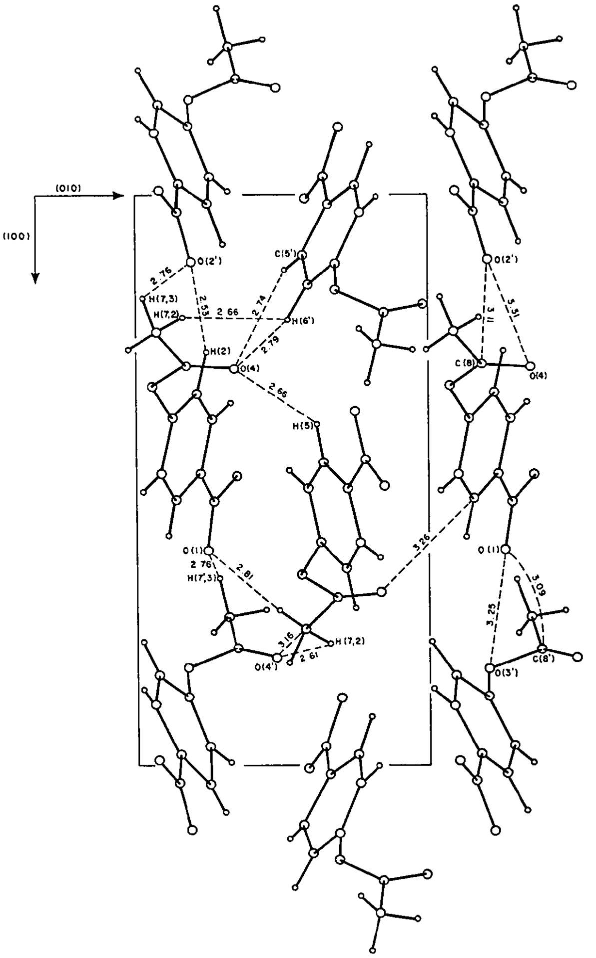


Fig. 3. Packing diagram in the [100] projection.

References

Barve, J. V. & Pant, L. M. (1971). *Acta Cryst.* **B27**, 1158.

Boyer, P. D., Lardy, H. & Myrback, K. (1960). *The Enzymes*, Vol. 4. New York: Academic Press.

Bryan, R. F. (1967). *J. Chem. Soc.* (*B*), p. 1311.

Busing, W. R. & Levy, H. A. (1964). *Acta Cryst.* **17**, 142.

Busing, W. R., Martin, K. O. & Levy, H. A. (1962). *ORFLS*. Report ORNL-TM-305, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

Chattaway, R. D. (1931). *J. Chem. Soc.* p. 2495.

Coppens, P. & Schmidt, G. M. J. (1965*a*). *Acta Cryst.* **18**, 654.

Coppens, P. & Schmidt, G. M. J. (1965*b*). *Acta Cryst.* **18**, 62.

Cromer, D. T. & Mann, J. B. (1968). *Acta Cryst.* **A24**, 321.

Germain, G. & Woolfson, M. M. (1968). *Acta Cryst.* **B24**, 91.

Kim, J. S., Chu, S. & Jeffrey, G. A. (1970). *Acta Cryst.* **B27**, 896.

Mak, T. C. W. & Trotter, J. (1965). *Acta Cryst.* **18**, 68.

Moore, F. H. (1963). *Acta Cryst.* **16**, 1169.

Tavale, S. S. & Pant, L. M. (1971). *Acta Cryst.* **B27**, 1479.

Trueblood, K. N., Goldish, E. & Donohue, J. (1961). *Acta Cryst.* **14**, 1009.