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The Crystal Structure of *p*-Bromoacetanilide

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The crystal structure of *p*-bromoacetanilide has been determined. The space group is $Pna2_1$ and the cell has dimensions $a=9{\cdot}70$, $b=13{\cdot}00$, $c=6{\cdot}67$ Å and contains 4 molecules. This compound is isostructural with the *p*-chloro derivative.

The crystal structure analysis of *p*-bromoacetanilide was in progress in this laboratory when the results of the study of *p*-chloroacetanilide were published (Subramanian, 1966). These compounds are isostructural; nevertheless, a comparison of the corresponding results of the two structural determinations is interesting.

Experimental

The unit-cell dimensions from rotation and Weissenberg photographs agree well with those given by Subramanian (1966) for the same compound (values in brackets):

Table 1. *Final atomic fractional coordinates* ($\times 10^4$) *and thermal parameters* ($\times 10$ Å^2) *with e.s.d.'s*

	x/a	*y/b*	*z/c*	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Br	2549±2	5415±1	−3075±3	46±1	52±1	50±2	0±2	0±2	0±3
O	4389±19	2614±20	5511±37	49±9	65±13	59±19	2±17	3±19	2±25
N	2230±29	2950±16	4688±34	41±8	40±9	48±17	1±13	0±16	1±20
C(1)	2449±12	4651±10	−640±20	32±7	37±8	34±15	1±12	1±15	−1±18
C(2)	1226±21	4299±19	71±34	46±10	54±12	53±23	−6±17	0±21	0±27
C(3)	1196±21	3770±12	1883±44	45±10	58±14	59±24	−1±19	0±22	−2±29
C(4)	2387±15	3492±14	2820±25	35±7	37±8	38±16	−4±12	−1±15	−1±18
C(5)	3609±14	3824±14	2057±40	37±8	45±10	43±17	0±14	0±17	−1±21
C(6)	3637±17	4428±16	302±36	38±8	40±9	45±18	−2±14	−1±17	−1±21
C(7)	3163±18	2511±21	5784±35	34±7	43±10	44±19	0±14	0±17	1±22
C(8)	2688±31	1911±23	7631±55	45±10	48±11	52±23	−1±17	3±21	1±26

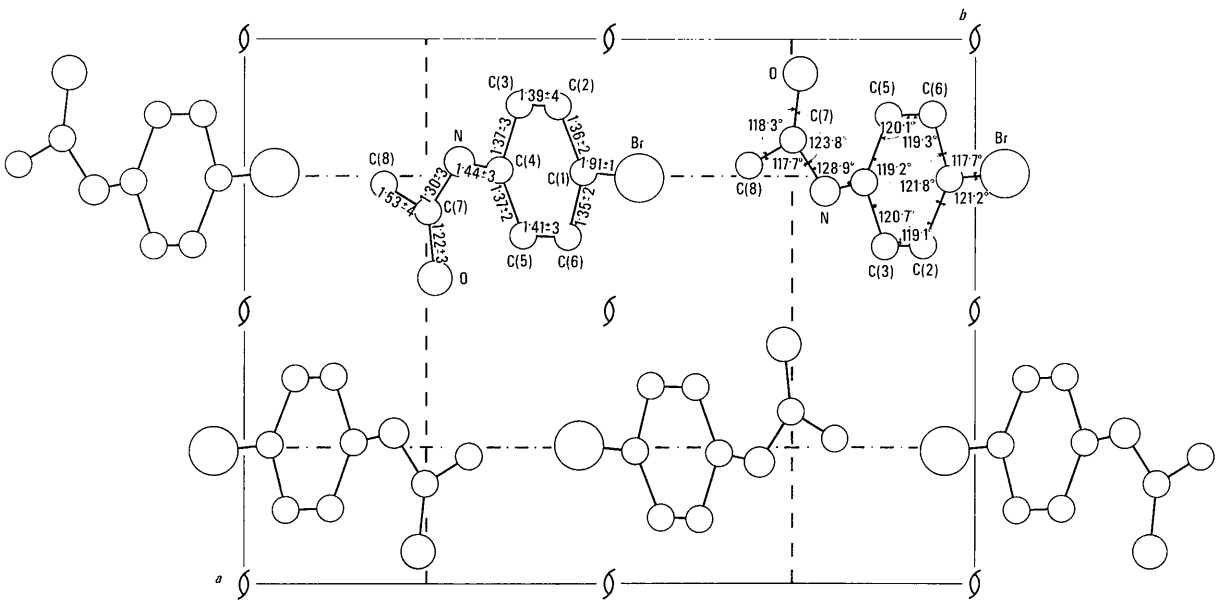

Fig. 1. Diagrammatic projection of the structure of *p*-bromoacetanilide along [001].

$BrONC_8H_8$ $M=216{\cdot}1$
$a=9{\cdot}70\pm1(9{\cdot}82)$, $b=13{\cdot}00\pm2(13{\cdot}02)$, $c=6{\cdot}67\pm2$ $(6{\cdot}72)$ Å
$V=845{\cdot}4$ Å^3, $Z=4$, $D_x=1{\cdot}70$ g.cm^{-3}
$\mu=68{\cdot}2$ (Cu $K\alpha$)

Space groups: $Pna2_1$ or $Pnam$ (from systematic absences).

The X-ray intensity data for Cu $K\alpha$ radiation were obtained photometrically from integrated multiple-film Weissenberg photographs taken around [001] up to $l=6$ and corrected for absorption, considering the sample as a cylinder with mean cross-section 0·016 cm. Corrections for the usual Lorentz, polarization and spot-shape effects were also applied. Approximate scaling was achieved first by Wilson's (1942) method

Table 2. *Observed and calculated structure factors*

A minus sign for F_o means 'less than'.

h	k	l	$10F_o$	$10F_c$	α
0	2	0	665	695	0
0	4	0	693	660	0
0	6	0	253	216	180
0	8	0	262	259	180
0	10	0	450	436	180
0	12	0	319	311	180
0	14	0	150	150	180
0	16	0	45-	18	180
1	0	0	27-	0	0
1	1	0	27-	4	0
1	2	0	197	166	0
1	3	0	45-	68	0
1	4	0	675	670	180
1	5	0	54-	53	0
1	6	0	731	707	180
1	7	0	64-	42	180
1	8	0	459	455	180
1	9	0	82-	17	0
1	10	0	82-	97	180
1	11	0	91-	45	180
1	12	0	82-	63	180
1	13	0	82-	3	180
1	14	0	73-	59	0
1	15	0	64-	16	180
1	16	0	45-	74	0
2	0	0	1957	2012	180
2	1	0	226	231	0
2	2	0	909	880	180
2	3	0	275	300	180
2	4	0	529	485	180
2	5	0	164-	166	0
2	6	0	169	185	180
2	7	0	73-	133	180
2	8	0	393	366	0
2	9	0	82-	64	0
2	10	0	337	315	0
2	11	0	91-	41	180
2	12	0	290	288	0
2	13	0	82-	26	0
2	14	0	122	133	0
2	15	0	64-	37	180
2	16	0	45-	53	0
3	0	0	45-	0	0
3	1	0	45-	69	180
3	2	0	736	647	0
3	3	0	178	211	180
3	4	0	918	840	0
3	5	0	64-	99	0
3	6	0	665	610	0
3	7	0	73-	33	180
3	8	0	337	302	0
3	9	0	82-	48	0
3	10	0	159	142	0
3	11	0	82-	37	0
3	12	0	82-	3	180
3	13	0	73-	29	0
3	14	0	94	96	180
3	15	0	54-	13	0
3	16	0	36-	83	180
4	0	0	890	894	0
4	1	0	84	105	0
4	2	0	468	486	0
4	3	0	66	59	180
4	4	0	656	572	0
4	5	0	73-	103	0
4	6	0	253	235	0
4	7	0	82-	70	0
4	8	0	300	280	180
4	9	0	82-	27	0
4	10	0	262	239	180
4	11	0	82-	25	0
4	12	0	206	204	180
4	13	0	73	22	180
4	14	0	94	109	180
4	15	0	45-	22	0
5	0	0	64-	0	0
5	1	0	64-	84	0
5	2	0	403	449	180
5	3	0	143	164	0
5	4	0	665	664	180
5	5	0	73-	111	180
5	6	0	412	409	180
5	7	0	82-	24	0
5	8	0	262	266	180
5	9	0	91-	37	180
5	10	0	82	83	180
5	11	0	82-	26	180
5	12	0	73-	16	180
5	13	0	64-	4	180
5	14	0	66	96	0
5	15	0	36-	14	180
6	0	0	853	796	180
6	1	0	73-	38	0
6	2	0	450	443	180
6	3	0	150	160	180
6	4	0	262	288	180
6	5	0	82-	26	180
6	6	0	82-	91	180
6	7	0	82-	141	180
6	8	0	187	196	0
6	9	0	82-	20	180
6	10	0	178	190	0
6	11	0	73-	47	180
6	12	0	150	168	0
6	13	0	64-	41	0
6	14	0	47	70	0
7	0	0	82-	0	0
7	1	0	82-	6	180
7	2	0	82-	92	0
7	3	0	82-	133	180
7	4	0	272	274	0
7	5	0	82-	20	0
7	6	0	337	335	0
7	7	0	82-	0	0
7	8	0	150	163	0
7	9	0	82-	19	0
7	10	0	73-	70	0
7	11	0	73-	20	0
7	12	0	64-	17	0
7	13	0	45-	12	180
7	14	0	18-	31	180
8	0	0	562	525	0
8	1	0	82-	106	0
8	2	0	497	452	0
8	3	0	91-	95	0
8	4	0	91-	29	0
8	5	0	82-	86	0
8	6	0	82-	59	0
8	7	0	82-	47	0
8	8	0	178	158	180
8	9	0	73-	54	0
8	10	0	122	119	180
8	11	0	54-	16	0
8	12	0	122	138	180
8	13	0	18-	26	180
9	0	0	82-	0	0
9	1	0	82-	0	0
9	2	0	82-	27	180
9	3	0	82-	125	0
9	4	0	197	139	180
9	5	0	82-	19	180
9	6	0	197	199	180
9	7	0	73-	12	0
9	8	0	112	95	180
9	9	0	64-	36	180
9	10	0	54-	38	189
9	11	0	45-	10	180
10	0	0	309	289	180
10	1	0	82-	82	180
10	2	0	197	193	180
10	3	0	73-	12	180
10	4	0	73-	83	180
10	5	0	73-	74	180
10	6	0	64-	14	180
10	7	0	64-	15	180
10	8	0	54-	61	0
10	9	0	45-	48	180
10	10	0	77	85	0
11	0	0	64-	0	0
11	1	0	64-	44	180
11	2	0	103	71	0
11	3	0	64-	65	180
11	4	0	112	109	0
11	5	0	54-	24	0
11	6	0	84	94	0
11	7	0	45-	6	0
11	8	0	27-	44	0
12	0	0	56	92	0
12	1	0	45-	11	0
12	2	0	66	84	0
12	3	0	36-	3	0
12	4	0	36-	64	0
12	5	0	27-	31	0
0	1	1	451	502	215
0	3	1	1723	1742	135
0	5	1	570	552	147
0	7	1	683	648	140
0	9	1	404	376	167
0	11	1	73	98	159
0	13	1	99	104	331
0	15	1	39-	69	325
1	1	1	762	773	179
1	2	1	26-	47	262
1	3	1	1339	1215	184
1	4	1	32-	67	157
1	5	1	444	388	127
1	6	1	39-	24	176
1	7	1	252	229	341
1	8	1	45-	56	108
1	9	1	331	311	359
1	10	1	52-	15	302
1	11	1	278	279	346
1	12	1	52-	20	137
1	13	1	166	164	344
1	14	1	43	24	295
1	15	1	89-	99	352
1	16	1	26-	5	349
2	0	1	319	341	132
2	1	1	219	294	359
2	2	1	213	227	305
2	3	1	789	821	332
2	4	1	163	170	126
2	5	1	808	734	327
2	6	1	145-	153	273
2	7	1	616	543	336
2	8	1	45-	100	97
2	9	1	398	385	331
2	10	1	52-	60	311
2	11	1	52-	40	324
2	12	1	52-	51	93
2	13	1	66	62	183
2	14	1	46	16	284
2	15	1	39-	52	139
2	16	1	26-	3	90
3	1	1	1054	1061	334
3	2	1	119	112	322
3	3	1	749	785	356
3	4	1	39-	81	24
3	5	1	39-	21	270
3	6	1	45	124	306
3	7	1	152	164	130
3	8	1	52-	15	11
3	9	1	258	240	152
3	10	1	52-	29	303
3	11	1	278	270	166
3	12	1	52-	21	31
3	13	1	172	189	165
3	14	1	36	24	131
3	15	1	32-	75	195
3	16	1	19-	15	157
4	0	1	179	210	50
4	1	1	166	153	243
4	2	1	153	141	275
4	3	1	380	388	168
4	4	1	39-	74	25
4	5	1	590	585	162
4	6	1	45-	40	328
4	7	1	524	508	159
4	8	1	52-	51	201
4	9	1	311	298	146
4	10	1	52-	45	137
4	11	1	52-	51	73
4	12	1	52-	21	245
4	13	1	45-	49	50
4	14	1	39-	24	112
4	15	1	32-	26	311
5	1	1	795	782	154
5	2	1	99	121	128
5	3	1	490	512	176
5	4	1	45-	64	201
5	5	1	45-	51	119
5	6	1	52-	97	144
5	7	1	146	168	306
5	8	1	52-	47	218
5	9	1	146	154	337
5	10	1	52-	20	151
5	11	1	192	226	340
5	12	1	45-	17	190
5	13	1	126	146	351
5	14	1	32-	16	339
5	15	1	19-	58	6
6	0	1	212	235	164
6	1	1	152	136	1
6	2	1	45-	11	110
6	3	1	384	376	333
6	4	1	106	117	122
6	5	1	384	400	333
6	6	1	52-	55	274
6	7	1	285	326	335
6	8	1	52-	50	56
6	9	1	205	226	332
6	10	1	52-	81	294
6	11	1	45-	19	270
6	12	1	45-	22	15
6	13	1	39-	29	206
6	14	1	26-	33	297
7	1	1	371	361	351
7	2	1	52-	22	289
7	3	1	398	392	354
7	4	1	52-	61	28
7	5	1	93	103	330
7	6	1	52-	101	351
7	7	1	52-	90	171
7	8	1	52-	46	11
7	9	1	152	142	167
7	10	1	45-	2	135
7	11	1	126	123	170
7	12	1	39-	19	320
7	13	1	86	90	165
8	0	1	192	171	355
8	1	1	272	226	139
8	2	1	93	111	294
8	3	1	278	261	157
8	4	1	52-	11	149
8	5	1	338	313	135
8	6	1	52-	23	25
8	7	1	159	149	159
8	8	1	52-	22	162
8	9	1	179	171	151
8	10	1	39-	40	117
8	11	1	39-	17	229
8	12	1	26-	33	168
9	1	1	199	198	177
9	2	1	52-	15	130
9	3	1	239	232	174
9	4	1	52-	57	216
9	5	1	86	78	158
9	6	1	52-	98	156
9	7	1	86	60	10
9	8	1	45-	25	200
9	9	1	99	90	351
9	10	1	32-	15	98
9	11	1	66	71	354
10	0	1	93	84	200
10	1	1	73	66	339
10	2	1	93	86	115
10	3	1	172	152	332
10	4	1	45-	28	270
10	5	1	152	143	325
10	6	1	39-	35	154
10	7	1	133	115	328
10	8	1	32-	30	337
10	9	1	73	79	334
10	10	1	13-	13	356
11	1	1	166	140	343
11	2	1	39-	39	325
11	3	1	106	102	351
11	4	1	39-	40	353
11	5	1	32-	23	12
11	6	1	32-	47	331
11	7	1	26-	28	156
11	8	1	13-	13	343
12	0	1	53	38	23
12	1	1	26-	14	196
12	2	1	26-	25	309
12	3	1	26-	49	170
12	4	1	19-	17	344
0	2	2	703	737	148
0	4	2	404	366	54
0	6	2	415	362	216
0	8	2	103	78	346
0	10	2	298	274	304
0	12	2	211	206	327
0	14	2	127	129	314
0	16	2	21-	33	15
1	1	2	48-	56	117
1	2	2	602	531	329
1	3	2	30-	34	172
1	4	2	773	720	322
1	5	2	37-	69	41
1	6	2	1087	1045	330
1	7	2	42-	49	268
1	8	2	437	421	306
1	9	2	49-	5	31
1	10	2	171	146	307
1	11	2	51-	30	218
1	12	2	49-	22	340
1	13	2	46-	10	5
1	14	2	103	85	162
1	15	2	31-	5	239
1	16	2	21-	52	143
2	0	2	855	899	333
2	1	2	156	192	63
2	2	2	722	693	310
2	3	2	136	175	235
2	4	2	342	273	308
2	5	2	191	170	40
2	6	2	83	70	43
2	7	2	44-	69	258
2	8	2	198	181	139
2	9	2	49-	104	13
2	10	2	294	291	143
2	11	2	49-	54	212
2	12	2	158	153	137
2	13	2	44-	10	90
2	14	2	94	102	133
2	15	2	30-	18	213
2	16	2	17-	22	168
3	1	2	96	123	305
3	2	2	545	591	128
3	3	2	35-	28	272
3	4	2	538	538	129
3	5	2	40-	16	288
3	6	2	628	634	140
3	7	2	46-	48	153
3	8	2	365	353	133
3	9	2	49-	46	29
3	10	2	255	225	138
3	11	2	49-	18	109
3	12	2	47-	92	183
3	13	2	42-	20	123
3	14	2	96	89	354
3	15	2	26-	6	180
4	0	2	606	637	163
4	1	2	94	136	347
4	2	2	580	613	144
4	3	2	107	143	173
4	4	2	338	341	132
4	5	2	44-	48	131
4	6	2	46-	5	324
4	7	2	47-	64	139
4	8	2	320	284	333
4	9	2	49-	51	180
4	10	2	255	268	331
4	11	2	49-	38	11
4	12	2	105	100	312
4	13	2	39-	4	256
4	14	2	59	63	306
4	15	2	23-	5	31
5	1	2	107	114	123
5	2	2	446	418	311
5	3	2	72	43	180
5	4	2	393	422	304
5	5	2	46-	45	153
5	6	2	417	456	323
5	7	2	49-	30	353
5	8	2	277	273	305
5	9	2	51-	10	236
5	10	2	165	189	328
5	11	2	46-	44	329
5	12	2	42-	63	355
5	13	2	35-	28	327
5	14	2	68	64	142
6	0	2	461	444	329
6	1	2	50	78	72
6	2	2	426	396	318
6	3	2	130	117	295
6	4	2	169	163	310
6	5	2	103	72	347
6	6	2	22-	38	7
6	7	2	51-	80	237
6	8	2	136	144	143
6	9	2	49-	68	7
6	10	2	145	166	150
6	11	2	42-	33	159
6	12	2	101	97	131
6	13	2	30-	19	24
6	14	2	19-	49	140
7	1	2	88	81	314
7	2	2	220	199	139
7	3	2	68	93	354
7	4	2	369	336	144
7	5	2	51-	66	311
7	6	2	413	391	144
7	7	2	49-	45	158
7	8	2	209	200	132
7	9	2	46-	35	167
7	10	2	70	75	124
7	11	2	37-	38	145
7	12	2	30	17	180
7	13	2	21-	22	162
8	0	2	365	333	152
8	1	2	51-	29	38
8	2	2	268	236	108
8	3	2	105	90	151
8	4	2	61	74	176
8	5	2	49-	42	81
8	6	2	49-	15	133
8	7	2	46-	15	50
8	8	2	59	69	257
8	9	2	40-	58	161
8	10	2	107	87	334
8	11	2	30-	4	26
8	12	2	90	82	306
9	1	2	72	68	137
9	2	2	125	102	321
9	3	2	47-	64	154
9	4	2	250	214	328
9	5	2	46-	39	137
9	6	2	277	244	329
9	7	2	40-	50	349
9	8	2	132	132	313
9	9	2	31-	25	289
9	10	2	26-	39	298
9	11	2	15-	21	330
10	0	2	202	172	323
10	1	2	44-	43	211
10	2	2	143	121	313
10	3	2	89	65	47
10	4	2	42	47	301
10	5	2	39-	40	272
10	6	2	35-	16	32
10	7	2	31-	30	3
10	8	2	57	41	128
10	9	2	19-	38	326
11	1	2	86	56	301
11	2	2	90	68	126
11	3	2	48	27	337
11	4	2	118	106	137
11	5	2	28-	10	276
11	6	2	79	98	142
11	7	2	15-	12	142
12	0	2	79	83	155
12	1	2	21-	9	348
12	2	2	55	60	146
12	3	2	15-	27	184
0	1	3	549	501	309
0	3	3	373	323	315
0	5	3	608	555	309
0	7	3	316	284	285
0	9	3	386	381	326
0	11	3	149	149	267
0	13	3	37-	31	47
0	15	3	47	73	117
1	1	3	799	790	284
1	2	3	25-	31	334
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1	6	3	37-	26	328
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1	9	3	338	340	105
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1	14	3	31-	13	293
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2	1	3	163	180	98
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2	4	3	37	82	224
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2	11	3	112	94	85
2	12	3	41-	43	121
2	13	3	36-	42	268
2	14	3	29-	13	0
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6	13	3	20-	27	301
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7	7	3	107	84	314
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7	9	3	137	134	284
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7	11	3	89	104	292
7	12	3	22-	20	273
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8	1	3	44-	40	261
8	2	3	44-	26	128
8	3	3	235	222	320
8	4	3	43-	20	76
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8	10	3	27-	17	23
8	11	3	49	66	302
9	1	3	221	204	285
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11	5	3	17-	24	82
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1	8	4	222	285	96
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7	8	4	70-	126	274
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10	4	4	50-	39	90
10	5	4	44-	26	90
10	6	4	35-	2	270
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11	2	4	26-	47	277
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0	7	5	204	176	78
0	9	5	159	151	59
0	11	5	58	31	57
0	13	5	42	39	328
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1	2	5	36-	14	161
1	3	5	271	235	98
1	4	5	43-	29	180
1	5	5	201	181	73
1	6	5	47-	16	37
1	7	5	65	67	226
1	8	5	49-	16	155
1	9	5	143	152	255
1	10	5	44-	15	56
1	11	5	129	119	252
1	12	5	33-	2	135
1	13	5	57	72	260
2	0	5	37-	32	216
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2	11	5	46	34	232
2	12	5	31-	17	177
2	13	5	23	16	151
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5	10	5	34-	13	57
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5	12	5	11-	8	234
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6	7	5	151	152	246
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6	9	5	72	54	243
6	10	5	27-	10	270
6	11	5	17-	31	232
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7	3	5	122	111	276
7	4	5	43-	17	253
7	5	5	78	71	254
7	6	5	38-	39	247
7	7	5	36-	24	48
7	8	5	31-	21	284
7	9	5	71	68	78
7	10	5	14-	11	206
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8	1	5	41-	40	121
8	2	5	40-	50	242
8	3	5	151	145	72
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8	5	5	109	108	82
8	6	5	31-	19	68
8	7	5	100	91	59
8	8	5	21-	13	134
9	1	5	103	99	73
9	2	5	33-	12	85
9	3	5	83	74	92
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1	5	6	68-	10	29
1	6	6	230	216	241
1	7	6	70-	16	292
1	8	6	169	172	231
1	9	6	62-	7	172
1	10	6	81	71	224
1	11	6	44-	11	270
1	12	6	22-	3	71
2	0	6	144	154	232
2	1	6	59-	65	139
2	2	6	277	254	240
2	3	6	65-	7	321
2	4	6	123	91	236
2	5	6	70-	29	148
2	6	6	70-	24	70
2	7	6	66-	26	314
2	8	6	68	64	50
2	9	6	60-	6	142
2	10	6	93	72	64
2	11	6	41-	7	345
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3	2	6	164	199	61
3	3	6	66-	11	175
3	4	6	199	220	44
3	5	6	70-	13	154
3	6	6	171	183	59
3	7	6	67-	10	96
3	8	6	123	142	49
3	9	6	56-	12	41
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3	11	6	33-	13	67
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4	2	6	166	160	63
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4	9	6	51-	9	58
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5	1	6	70-	47	44
5	2	6	176	162	241
5	3	6	66-	7	310
5	4	6	171	152	229
5	5	6	65-	20	99
5	6	6	126	136	234
5	7	6	57-	4	256
5	8	6	101	116	234
5	9	6	43-	10	209
5	10	6	25-	52	233
6	0	6	134	105	227
6	1	6	67-	26	145
6	2	6	114	114	242
6	3	6	65-	52	299
6	4	6	106	82	236
6	5	6	59-	29	219
6	6	6	56-	26	40
6	7	6	49-	20	243
6	8	6	41-	29	72
6	9	6	24-	5	201
7	1	6	60-	23	214
7	2	6	61	64	67
7	3	6	57-	7	147
7	4	6	103	95	50
7	5	6	49-	33	270
7	6	6	84	102	56
7	7	6	35-	7	106
8	0	6	94	104	45
8	1	6	48-	10	5
8	2	6	86	56	68
8	3	6	44-	29	74
8	4	6	40-	32	25
8	5	6	32-	21	68
9	1	6	24-	26	67

Table 3. *Comparison of bond distances and angles in p-bromoacetanilide and in p-chloroacetanilide (values in brackets)*

Br —C(1)	1·91 ± 1 Å		Br —C(1)–C(2)	121·2 ± 1·2°	
C(1)–C(2)	1·36 ± 2	(1·40 ± 3 Å)	Br —C(1)–C(6)	117·7 ± 1·2	
C(2)–C(3)	1·39 ± 4	(1·36 ± 3)	C(1)–C(2)–C(3)	119·1 ± 1·8	(117 ± 3°)
C(3)–C(4)	1·37 ± 3	(1·48 ± 3)	C(2)–C(3)–C(4)	120·7 ± 1·9	(122 ± 3)
C(4)–C(5)	1·37 ± 2	(1·45 ± 3)	C(3)–C(4)–C(5)	119·2 ± 1·8	(116 ± 3)
C(5)–C(6)	1·41 ± 3	(1·41 ± 3)	C(4)–C(5)–C(6)	120·1 ± 1·6	(122 ± 3)
C(6)–C(1)	1·35 ± 2	(1·38 ± 3)	C(5)–C(6)–C(1)	119·3 ± 1·5	(117 ± 3)
C(4)–N	1·44 ± 3	(1·34 ± 3)	C(6)–C(1)–C(2)	121·8 ± 1·6	(126 ± 3)
N—C(7)	1·30 ± 3	(1·43 ± 3)	C(5)–C(4)–N	124·7 ± 1·9	(126 ± 3)
C(7)–O	1·22 ± 3	(1·22 ± 3)	C(3)–C(4)–N	115·8 ± 1·9	(117 ± 3)
C(7)–C(8)	1·53 ± 4	(1·60 ± 3)	C(4)–N—C(7)	128·9 ± 2·3	(127 ± 3)
			N—C(7)–O	123·8 ± 2·5	(121 ± 3)
			N—C(7)–C(8)	117·7 ± 2·0	(114 ± 3)
			O—C(7)–C(8)	118·3 ± 2·3	(126 ± 3)

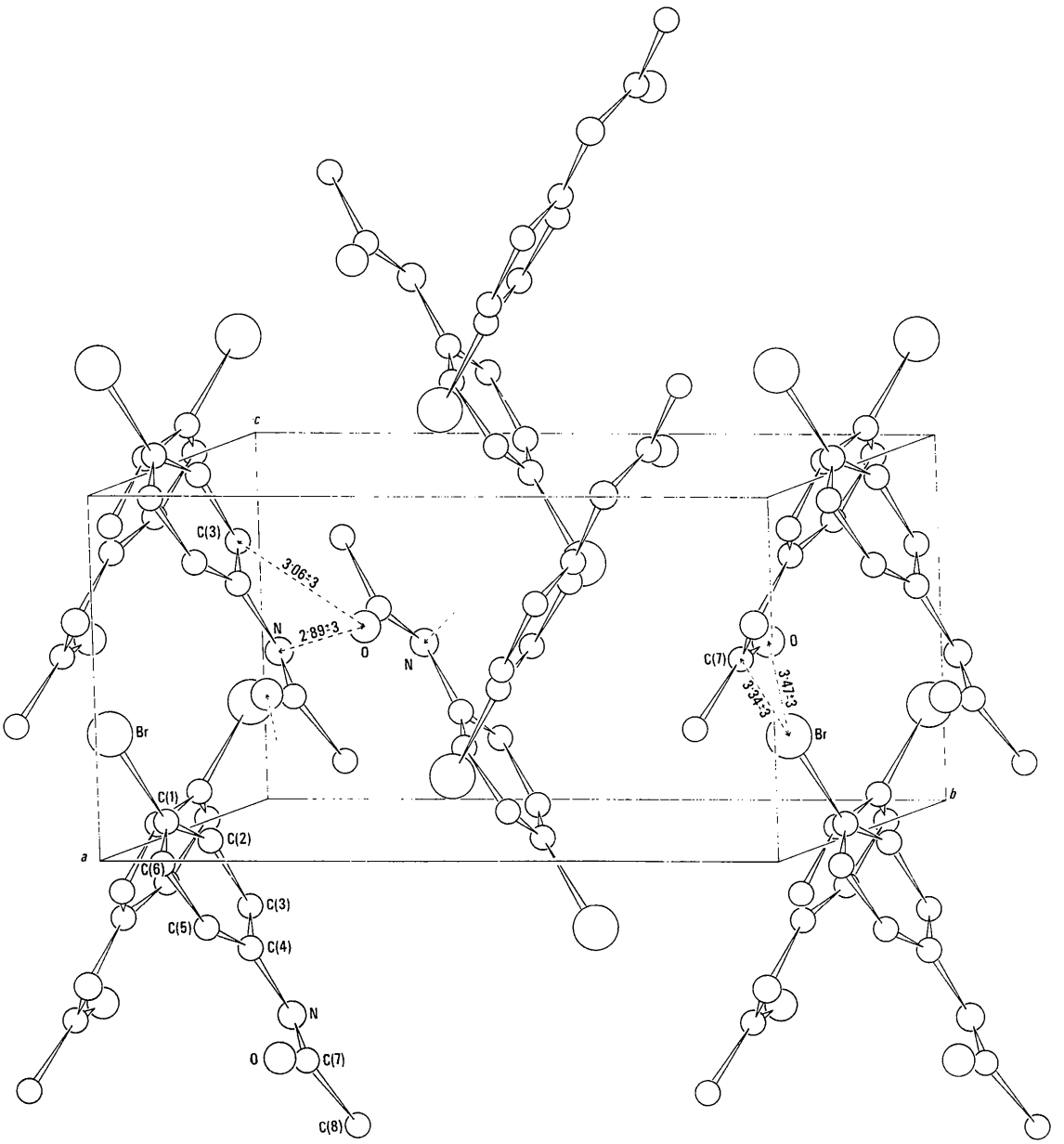

Fig. 2. Clinographic projection of the structure of *p*-bromoacetanilide.

applied to each layer. The disorder effects observed by Subramanian for his crystals were not apparent in the Weissenberg photographs of our crystals. The atomic coordinates and the $Pna2_1$ space group found for *p*-chloroacetanilide by Subramanian were used as starting parameters which were refined with the use of Booth's differential synthesis and anisotropic thermal parameters. At the end of the refinement the residual error factors (R, for observed reflexions only; R', assuming $F_o=\frac{1}{2}F_{\min}$ when $F_c \geq F_{\min}$ for unobserved reflexions; multiplicities not considered) were $R=8{\cdot}2\%$, $R'=14{\cdot}8\%$. The final coordinates and anisotropic thermal parameters with their e.s.d.'s are reported in Table 1. No attempt was made to locate the hydrogen atoms directly. In Table 2 observed and calculated structure factors are compared. The scattering factors used are those of Thomas & Umeda (1957) for Br and of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for O, N and C.

Discussion

The bond lengths and angles observed in the molecule are shown in Fig. 1 and compared in Table 3 with the corresponding values found by Subramanian in *p*-chloroacetanilide.

Comparing these values it appears that the geometry of the molecule is not significantly changed by substituting bromine for chlorine. The acetyl group in the Br derivative has dimensions which agree better with those generally found in *N*-substituted amides [*e.g.* acetanilide (Brown & Corbridge, 1954), *N*-acetyl-α-D-glucosamide (Johnson, 1966)]. Nevertheless, the e.s.d.'s are not small enough to allow any sensible discussion of the nature of the bonds. As found in the chlorine derivative, the halogenobenzene group is planar, the least-squares plane being

$$-0{\cdot}0633x+0{\cdot}8476y+0{\cdot}5269z=4{\cdot}7288\ .$$

The acetyl group is also planar:

$$0{\cdot}0266x+0{\cdot}8248y+0{\cdot}5648z=4{\cdot}9814\ .$$

The dihedral angle between these planes is 5·8° which agrees well with the value 5° found in *p*-chloroacetanilide. The oxygen atom is 0·18 Å out of the benzene plane. This distortion and the enlargement of the angle C(4)–N–C(7) = 128·9° ± 2·3° from the trigonal value can be attributed to steric hindrance from the O and C(5) atoms (O–C(5) = 2·89 ± 3 Å), as observed also in the Cl derivative (2·83 ± 3 Å). The packing (Fig. 2) is determined by the hydrogen bond $N^{ii}H\cdots O$ (2·87 ± 3 Å) forming a chain almost parallel to the [100] axis. The $O^{iii}\cdots C(3)$ = 3·06 ± 3 Å distance is just a little longer than the sum of van der Waals radii (2·84 Å). Other distances less than 3·5 Å are as follows:

$Br\cdots N^{i}$	= 3·47 Å	i $\frac{1}{2}-x, \frac{1}{2}+y, \bar{z}$
$Br\cdots C(7^{i})$	= 3·34	ii $\frac{1}{2}+x, \frac{1}{2}-y, 1-z$
$O\cdots C(4^{ii})$	= 3·44	iii $x-\frac{1}{2}, \frac{1}{2}-y, 1-z$.

All the calculations were performed on the Olivetti Elea 6001/S computer of the Centro di Calcolo Elettronico dell'Università di Parma with the programs of Nardelli, Musatti, Domiano & Andreetti (1964, 1965). The authors are indebted to the Consiglio Nazionale delle Ricerche for financial support.

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