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Crystal and Molecular Structure of *s*-Triphenyltriazine

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The structure of *s*-triphenyltriazine was refined by three-dimensional differential Fourier synthesis. The crystals are monoclinic, space group $P2_1/c$, with four molecules in a cell with dimensions:

$$a = 10{\cdot}94,\ b = 3{\cdot}91,\ c = 35{\cdot}84\ \text{Å};\ \beta = 90°\ 38'.$$

The molecule is not planar. The planes passing through the three phenyl groups are tilted by angles of 7·6°, 10·9° and 6·9° with respect to the plane passing through the triazine ring. The sense of twist of one phenyl group is opposite to that of the other two. The bonds connecting the phenyl groups to the central ring are not exactly in the plane passing through the atoms of the triazine group. The great average length of these bonds ($1{\cdot}47_5$ Å, with an estimated standard deviation of 0·007 Å) and the deviation of the molecule from planarity indicate that the phenyl groups are, at least, not completely conjugated with the triazine ring. The geometry of the molecule is compared with that of other compounds which show steric inhibition of resonance.

Introduction

The crystal and molecular structures of several azines have been investigated in recent years and interesting correlations with their electronic structures have been established. In order to obtain further information on this class of compound and to examine the influence of substituents on the structure as well as on the molecular conformation a study of *s*-triphenyltriazine was undertaken. Preliminary results on the crystal structure were previously reported (Giglio & Ripamonti, 1959). In this paper the results of a detailed three-dimensional analysis are reported. These results allowed us to reach some conclusions not only on the bond angles and bond lengths in the molecule but also on the deviation from planarity due to the tilting of the phenyl groups with respect to the triazine ring. A comparison with the molecular geometry of the isosteric compound 1,3,5-triphenylbenzene (Farag, 1954) appears of particular interest in this respect.

Experimental

s-Triphenyltriazine crystallizes from toluene as transparent well formed monoclinic prisms, elongated along **b**.

From precession photographs taken with Cu $K\alpha$ radiation the unit cell parameters were found to be

$$a = 10{\cdot}94, \quad b = 3{\cdot}91, \quad c = 35{\cdot}84\ \text{Å}; \quad \beta = 90°38'.$$

The space group indicated by the systematic absences is $P2_1/c$ (C_{2h}^5). Four molecules per unit cell give a calculated density of 1·326 g.cm^{-3}.

Intensity data were collected with Cu $K\alpha$ radiation using multiple-film equi-inclination Weissenberg photographs about **b** for layer lines 0 to 2. The zero-layer about the *a* axis was recorded to provide cross-correlation of the *b*-axis data.

Care was taken to chose crystals having regular shapes (cross-section of about 0,2 × 0,2 mm).

The number of independent reflexions observed was 1152. The intensities were measured by eye-estimation, corrected for change of spot shape on upper layer equi-inclination photographs (Phillips, 1954) and reduced to structure amplitudes by a data reduction program written for an IBM 1620 computer (Damiani, De Santis, Giglio & Ripamonti, 1962). No corrections were made for absorption and there was no evidence of extinction.

Structure determination

The structure projected on (010) had been previously determined (Giglio & Ripamonti, 1959). The molecular orientation was deduced by inspection of the section *h*0*l* of the weighted reciprocal lattice, which showed the characteristic Fourier transform of a benzene ring, whereas its location with respect to the origin was established with the aid of a modified Patterson function (Giglio, Liquori & Ripamonti, 1958). The *x* and *z* coordinates were then refined by Fourier synthesis and structure factor calculations until R_{h0l} was reduced to 0·15. Assuming a planar model with normal bond lengths and bond angles the projection of the molecule on the (100) plane was deduced. The molecule was then moved along the *b* axis until a reasonable *R* index was obtained for the 0*kl* reflexions. Successive structure factors, Fourier and difference Fourier calculations reduced *R* to 0·20.

The three-dimensional structure factors, calculated with the atomic coordinates thus obtained, gave $R =$ 0·29. A three-dimensional Fourier synthesis was then computed, with a program written for the IBM 1620

Table 1. *Comparison between final observed and calculated structure factors*

Values are multiplied by 10.

H	K	L	FOBS	FCAL
1	0	0	939	792
2	0	0	1071	-872
3	0	0	139	71
4	0	0	492	-376
5	0	0	53	-47
6	0	0	431	343
7	0	0	538	441
8	0	0	34	-29
9	0	0	127	-185
10	0	0	228	281
11	0	0	313	362
14	0	0	57	-115
1	0	2	158	137
-1	0	2	183	-155
2	0	2	947	828
-2	0	2	743	-777
4	0	2	141	89
-4	0	2	64	-43
5	0	2	944	-883
-5	0	2	944	846
6	0	2	582	-485
-6	0	2	496	391
7	0	2	117	99
-7	0	2	90	-60
8	0	2	128	-102
-8	0	2	160	147
9	0	2	141	-138
-9	0	2	137	144
12	0	2	73	74
-12	0	2	44	-67
0	0	4	693	-599
1	0	4	274	-281
-1	0	4	349	-355
2	0	4	917	-788
-2	0	4	741	-699
3	0	4	65	63
-3	0	4	140	108
4	0	4	504	-373
-4	0	4	542	-490
5	0	4	518	-422
-5	0	4	466	-373
6	0	4	441	334
-6	0	4	469	359
8	0	4	120	-136
-8	0	4	118	-119
10	0	4	59	-34
11	0	4	69	-67
-12	0	4	38	-63
13	0	4	46	-37
-13	0	4	47	-35
0	0	6	174	-205
1	0	6	1255	1292
-1	0	6	1034	-1033
2	0	6	235	-197
-2	0	6	301	279
3	0	6	276	203
-3	0	6	413	-321
4	0	6	270	223
-4	0	6	235	-200
5	0	6	205	163
-5	0	6	186	-131
6	0	6	34	21
-6	0	6	52	-51
7	0	6	69	45
-7	0	6	60	-56
9	0	6	66	55
-10	0	6	53	67
11	0	6	50	68
-11	0	6	99	-116
12	0	6	69	77
-12	0	6	42	-44
13	0	6	53	-51
-13	0	6	55	63
0	0	8	917	891
1	0	8	167	193
-1	0	8	134	169
2	0	8	34	36
3	0	8	317	-278
-3	0	8	406	-328
4	0	8	90	-78
-4	0	8	51	-39
5	0	8	90	76
-5	0	8	74	63
6	0	8	39	28
-6	0	8	38	47
7	0	8	95	-94
-7	0	8	169	-134
8	0	8	174	-161
-8	0	8	146	-131
11	0	8	47	60
-11	0	8	64	57
0	0	10	54	-2
1	0	10	41	28
-1	0	10	77	81
2	0	10	252	-230
-2	0	10	184	184
3	0	10	321	256
-3	0	10	408	-333
4	0	10	168	145
-4	0	10	65	52
5	0	10	283	-273
-5	0	10	167	145
6	0	10	123	72
-6	0	10	148	-109
7	0	10	218	-184
-7	0	10	335	321
8	0	10	58	-31
-8	0	10	90	-65
9	0	10	272	245
-9	0	10	294	-267
10	0	10	163	158
-10	0	10	85	-82
12	0	10	60	80
-12	0	10	106	-120
13	0	10	64	81
0	0	12	329	369
1	0	12	135	132
-1	0	12	24	23
2	0	12	253	-226
-2	0	12	200	-196
3	0	12	470	396
-3	0	12	498	521
4	0	12	396	344
-4	0	12	221	194
5	0	12	90	77
-5	0	12	29	16
6	0	12	50	-54
-6	0	12	36	36
7	0	12	354	310
-7	0	12	382	392
8	0	12	216	177
-8	0	12	137	117
9	0	12	194	-196
10	0	12	200	203
-10	0	12	200	181
11	0	12	45	78
-12	0	12	62	49
-13	0	12	32	-29
0	0	14	92	84
1	0	14	439	-443
-1	0	14	473	476
2	0	14	91	102
-2	0	14	472	-456
3	0	14	613	500
-3	0	14	524	-507
4	0	14	215	177
-4	0	14	97	-85
5	0	14	34	22
6	0	14	102	-80
-6	0	14	62	69
7	0	14	131	-99
-7	0	14	349	317
8	0	14	753	-647
-8	0	14	680	637
9	0	14	164	-144
-9	0	14	122	-127
10	0	14	197	187
-10	0	14	143	-158
13	0	14	63	-120
-13	0	14	165	184
0	0	16	106	-109
1	0	16	75	-73
-1	0	16	233	-250
2	0	16	545	-556
-2	0	16	815	-855
3	0	16	907	-904
-3	0	16	549	-511
4	0	16	249	200
-4	0	16	312	272
5	0	16	146	98
6	0	16	248	254
-6	0	16	484	505
7	0	16	211	187
-7	0	16	204	-183
8	0	16	727	-651
-8	0	16	929	-869
9	0	16	515	-469
-9	0	16	250	-249
10	0	16	90	-90
11	0	16	46	65
13	0	16	102	156
-13	0	16	156	188
0	0	18	53	-50
1	0	18	172	179
-1	0	18	125	-128
2	0	18	172	-164
-2	0	18	398	417
3	0	18	298	-259
-3	0	18	207	192
4	0	18	55	-51
-4	0	18	49	52
5	0	18	60	-44
6	0	18	123	127
-6	0	18	146	-141
-7	0	18	101	-78
8	0	18	545	476
-8	0	18	411	-433
9	0	18	225	230
10	0	18	119	-135
-10	0	18	63	66
-12	0	18	41	-44
0	0	20	173	203
1	0	20	101	113
2	0	20	104	-91
-2	0	20	165	-159
3	0	20	221	210
-3	0	20	398	362
4	0	20	305	266
-4	0	20	155	136
5	0	20	106	89
-5	0	20	39	-24
6	0	20	86	-90
-6	0	20	80	94
7	0	20	277	232
-7	0	20	374	365
8	0	20	232	211
9	0	20	225	-215
-9	0	20	74	-76
10	0	20	168	151
-10	0	20	183	193
11	0	20	85	95
-12	0	20	83	75
1	0	22	104	-109
2	0	22	127	105
-2	0	22	134	-144
3	0	22	46	49
-3	0	22	90	95
4	0	22	130	-126
-4	0	22	64	-54
5	0	22	190	172
-5	0	22	47	-66
7	0	22	50	42
-7	0	22	155	-140
8	0	22	53	-58
-8	0	22	186	177
9	0	22	170	-149
-9	0	22	114	112
10	0	22	68	-87
12	0	22	19	-15
-12	0	22	68	67
0	0	24	109	117
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-2	0	24	33	-58
3	0	24	131	-121
-3	0	24	127	-116
-4	0	24	135	156
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-5	0	24	49	43
7	0	24	38	-27
-7	0	24	120	-102
8	0	24	192	-187
-8	0	24	127	-144
0	0	26	207	234
1	0	26	401	-438
-1	0	26	225	246
2	0	26	153	-154
-3	0	26	137	160
4	0	26	78	-80
5	0	26	60	-60
6	0	26	44	57
10	0	26	32	28
-10	0	26	46	-40
-11	0	26	146	104
0	0	28	242	-273
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2	0	28	151	-155
-2	0	28	64	-70
3	0	28	52	-57
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5	0	28	113	-140
-5	0	28	44	-66
-10	0	28	46	-39
11	0	28	34	-52
-11	0	28	71	-52
0	0	30	142	153
1	0	30	65	-91
-1	0	30	197	189
2	0	30	279	-298
-2	0	30	93	102
-4	0	30	78	-99
5	0	30	195	207
-5	0	30	295	-366
6	0	30	263	276
-6	0	30	65	-63
-7	0	30	69	93
-8	0	30	59	-60
9	0	30	61	61
-9	0	30	177	-91
10	0	30	45	53
0	0	32	747	771
1	0	32	525	555
-1	0	32	61	-75
2	0	32	133	-140
3	0	32	69	-74
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5	0	32	30	-38
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-6	0	32	107	115
7	0	32	135	168
-7	0	32	74	84
8	0	32	41	62
-8	0	32	34	-47
9	0	32	107	-108
-10	0	32	235	199
1	0	34	197	-210
2	0	34	102	101
-2	0	34	129	-117
3	0	34	65	70
-4	0	34	43	54
5	0	34	109	-123
-5	0	34	146	162
6	0	34	137	-161
8	0	34	81	-56
-8	0	34	112	91
9	0	34	50	-39
0	0	36	141	-146
-1	0	36	64	-73
2	0	36	136	-151
3	0	36	88	-87
-4	0	36	150	-160
5	0	36	111	-138
6	0	36	83	68
-6	0	36	64	75
7	0	36	69	79
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8	0	36	36	-44
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5	0	38	41	54
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0	0	40	151	162
1	0	40	85	95
-3	0	40	76	-71
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-3	0	42	70	-49
4	0	42	127	91
5	0	42	48	-38
-6	0	42	26	48
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3	0	44	65	63
-3	0	44	81	75
0	0	46	55	62
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0	1	2	606	754
0	1	3	1106	1254
0	1	4	1100	-1214
0	1	5	820	987
0	1	6	480	-571
0	1	7	307	352
0	1	8	191	196
0	1	9	338	-417
0	1	10	216	246
0	1	11	123	-121
0	1	12	129	-141
0	1	13	200	190
0	1	15	230	218
0	1	17	139	134
0	1	18	190	-184
0	1	19	236	229
0	1	20	118	130
0	1	21	144	-146
0	1	26	153	146
0	1	27	389	418
0	1	28	426	477
0	1	29	256	270
0	1	30	275	-280
0	1	31	193	-185
0	1	35	171	173
0	1	37	131	118
0	1	38	118	-113
1	1	0	496	475
1	1	1	625	-680
-1	1	1	574	-489
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1	1	3	553	581
1	1	4	941	-1066
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1	1	5	845	862
-1	1	5	231	-250
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1	1	7	732	-801
1	1	8	123	137
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1	1	13	213	234
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1	1	14	269	275
-1	1	14	253	-257
1	1	15	99	97
-1	1	15	117	123
1	1	17	75	82
-1	1	17	181	176
1	1	18	136	141
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1	1	19	87	-101
-1	1	20	161	145
1	1	21	102	-100
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1	1	28	126	127
1	1	29	74	65
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1	1	32	186	179
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1	1	33	136	-125
-1	1	33	118	-109
1	1	34	182	181
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1	1	36	224	-218
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-2	1	3	333	401
2	1	4	448	439
-2	1	4	91	-53
-2	1	5	69	74
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2	1	7	337	-364
-2	1	7	188	-165
2	1	8	181	206
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-2	1	10	70	-63
2	1	11	243	-252
-2	1	11	111	-92
2	1	12	456	-478
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2	1	14	57	-68
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2	1	18	181	174
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-2	1	20	302	291
2	1	23	66	-50
2	1	24	78	-78
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2	1	31	106	-86
2	1	33	159	-156
2	1	34	156	168
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2	1	39	170	-118
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2	1	43	78	-53
2	1	44	76	-60
3	1	0	132	123
3	1	1	183	155
-3	1	1	191	187
3	1	2	157	115
-3	1	2	107	-76
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-3	1	7	225	202
3	1	8	316	334
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3	1	9	104	-110
-3	1	9	44	-51
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-3	1	11	599	-542
3	1	12	299	-286
-3	1	12	228	-185
3	1	13	333	-316
3	1	14	115	-104
-3	1	14	547	519
3	1	15	126	132
-3	1	15	347	329
3	1	17	239	244
-3	1	17	84	68
3	1	18	417	-409
-3	1	18	107	82
3	1	19	125	-125
-3	1	19	162	-144
3	1	20	109	113
3	1	21	279	-258
-3	1	22	141	121
3	1	23	68	-52
-3	1	24	134	-105
3	1	25	123	121
-3	1	25	108	92
3	1	26	83	-99
3	1	27	74	62
3	1	35	99	-102
3	1	37	65	65
3	1	40	78	75
4	1	0	238	-162
-4	1	1	166	-126
4	1	2	209	179
-4	1	2	142	103
4	1	3	211	178
-4	1	3	351	-325
4	1	4	154	125
-4	1	4	161	131
4	1	5	80	-70
-4	1	5	121	93
4	1	6	92	-75
-4	1	6	256	-210
4	1	8	80	68
-4	1	8	405	507
4	1	9	100	114
-4	1	11	131	-102
4	1	12	200	192
-4	1	12	136	108
-4	1	13	298	219
4	1	14	158	-162
4	1	15	89	107
-4	1	15	110	91
4	1	16	81	-97
-4	1	16	156	128
4	1	17	197	209
-4	1	17	130	117
4	1	18	202	-202
-4	1	18	105	85
4	1	19	99	85
-4	1	19	108	-89
4	1	20	66	71
4	1	21	139	-126
-4	1	21	99	78
4	1	22	80	-81
4	1	24	155	-181
-4	1	25	78	-57
-4	1	28	97	-109
-4	1	33	93	-92
-4	1	34	99	114
4	1	39	95	73
5	1	0	252	234
5	1	1	88	70
-5	1	1	452	-405
5	1	2	232	-198
-5	1	2	680	562
5	1	3	213	186
-5	1	3	419	-369
-5	1	4	250	199
-5	1	5	358	313
-5	1	6	75	-52
5	1	7	182	-173
-5	1	7	265	249
5	1	8	254	232
5	1	9	199	-198
-5	1	9	78	-74
5	1	10	74	-75
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6	1	17	81	-85
6	1	19	117	-96
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6	1	34	88	-124
6	1	35	107	81
6	1	36	64	-36
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7	1	4	230	-224
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7	1	7	114	107
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7	1	9	224	250
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-7	1	15	109	121
7	1	16	173	193
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-7	1	21	314	-273
-7	1	23	132	134
-7	1	24	86	-90
-7	1	25	105	72
-7	1	28	123	107
-8	1	1	140	-120
8	1	2	81	88
8	1	3	81	-62
-8	1	3	172	-189
8	1	4	91	-101
8	1	5	153	168
8	1	6	123	130
8	1	7	116	-113
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8	1	9	179	-165
-8	1	9	145	133
8	1	10	223	-242
8	1	11	343	-389
8	1	12	151	-161
-8	1	12	472	-475
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8	1	14	438	479
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8	1	18	106	113
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8	1	19	239	-263
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8	1	24	120	-129
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8	1	29	69	-83
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-9	1	3	95	-102
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-9	1	11	106	-96
9	1	12	130	-147
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9	1	13	102	-93
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9	1	14	137	-155
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9	1	19	281	-314
9	1	20	196	236
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10	1	14	131	-170
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10	1	17	113	131
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10	1	18	161	-199
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10	1	25	54	-64
10	1	27	92	98
10	1	28	51	60
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-11	1	1	71	-83
11	1	2	100	108
11	1	3	123	140
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0	2	1	135	-147
0	2	2	172	213
0	2	3	151	-164
0	2	4	137	-162
0	2	5	212	226
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0	2	7	151	-141
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0	2	11	104	-126
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0	2	13	142	159
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0	2	16	71	-85
0	2	17	68	-68
0	2	18	54	-84
0	2	19	76	-102
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0	2	22	296	298
0	2	23	95	81
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0	2	30	85	103
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1	2	16	59	52
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1	2	25	169	173
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-1	2	27	251	-267
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-1	2	29	90	-80
-1	2	30	101	-86
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1	2	40	99	81
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-2	2	1	124	112
2	2	2	136	-121
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2	2	10	209	-228
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2	2	20	60	62
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2	2	22	62	-49
2	2	23	74	82
-2	2	23	133	122
-2	2	24	209	-226
-2	2	25	121	-114

Table 1 (*cont.*)

H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL	H	K	L	FOBS	FCAL
-2	2	26	147	-157	-4	2	4	238	205	-5	2	11	167	-169	7	2	1	113	102	8	2	26	76	-56	0	1	14	24	30
-2	2	29	101	-91	4	2	5	60	-50	5	2	12	117	-132	7	2	2	81	59	-8	2	26	77	-87	0	1	16	35	37
-2	2	31	116	118	-4	2	5	183	154	-5	2	12	47	37	7	2	3	130	121	8	2	28	56	36	0	1	22	27	-40
2	2	36	55	-62	4	2	6	159	152	-5	2	13	68	-58	-7	2	3	108	-122	-8	2	28	41	-56	0	1	24	41	-55
2	2	37	139	133	-4	2	6	333	-306	5	2	14	102	-120	7	2	5	96	84	8	2	30	42	45	0	1	32	33	30
2	2	38	97	-89	4	2	7	39	-63	-5	2	14	78	-88	7	2	6	73	-39	-9	2	5	170	174	0	1	33	71	-75
2	2	39	76	-67	-4	2	7	118	108	-5	2	15	50	-41	7	2	7	303	-335	-9	2	8	188	-204	0	1	39	29	28
2	2	41	77	-62	4	2	8	40	-48	5	2	16	62	-82	-7	2	7	104	77	9	2	9	113	-130	0	1	40	47	50
3	2	0	247	220	-4	2	8	124	-109	-5	2	16	95	-92	7	2	9	293	323	-9	2	9	258	-272	0	1	41	53	-65
3	2	1	279	-294	4	2	9	50	-46	5	2	17	51	50	7	2	10	335	376	9	2	10	84	-80	0	1	42	29	33
3	2	2	250	233	-4	2	10	352	351	-5	2	17	156	159	7	2	11	244	258	9	2	11	64	78	0	2	0	18	35
-3	2	2	263	248	4	2	11	75	-77	5	2	18	52	-50	-7	2	11	83	-88	-9	2	11	247	197	0	2	12	43	41
3	2	4	186	166	-4	2	11	97	99	-5	2	18	111	-120	7	2	12	100	118	-9	2	12	118	129	0	2	17	64	-68
3	2	5	200	-190	-4	2	12	53	52	-5	2	20	181	-197	7	2	13	76	-53	-9	2	14	64	72	0	2	18	59	-84
-3	2	5	275	-258	4	2	13	55	28	5	2	21	54	69	7	2	15	66	-53	9	2	15	72	-60	0	2	20	67	75
3	2	6	125	-103	-4	2	13	95	85	-5	2	21	111	128	7	2	18	66	55	9	2	20	140	144	0	2	21	60	78
-3	2	6	48	56	4	2	14	65	74	5	2	22	66	65	-7	2	18	66	-50	9	2	21	124	-118	0	2	26	68	-77
3	2	7	123	131	-4	2	14	56	-46	-5	2	22	66	-65	-7	2	19	108	104	9	2	22	90	-99	0	2	30	88	103
-3	2	7	127	-108	4	2	15	47	42	5	2	23	67	-51	-7	2	20	111	126	9	2	23	141	173	0	2	31	40	36
3	2	8	136	-140	4	2	16	48	-50	5	2	24	66	-66	-7	2	21	315	-267	9	2	24	109	-133	0	3	2	55	45
-3	2	8	123	-108	4	2	18	71	-68	-5	2	24	111	104	-7	2	22	313	255	-9	2	24	41	-46	0	3	4	29	-35
3	2	9	166	-171	4	2	19	62	-77	5	2	25	85	-123	-7	2	23	111	-89	-9	2	25	56	49	0	3	7	46	48
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3	2	10	146	162	4	2	22	209	244	5	2	26	123	-157	-7	2	26	134	-98	9	2	27	78	-74	0	3	11	57	-67
-3	2	10	365	357	-4	2	22	75	-72	5	2	28	64	68	7	2	29	81	72	9	2	28	60	76	0	3	12	40	-39
-3	2	11	190	179	-4	2	23	65	42	6	2	1	119	-101	-7	2	29	99	-98	9	2	29	46	-73	0	3	13	85	-95
-3	2	13	41	-44	4	2	24	115	-141	-6	2	2	81	59	-7	2	31	57	-65	-10	2	3	63	-68	0	3	14	31	-13
3	2	14	68	-79	4	2	26	76	-87	6	2	3	102	106	7	2	36	43	18	-10	2	4	72	-91	0	3	17	89	85
3	2	15	118	-114	4	2	30	68	81	-6	2	4	74	-64	8	2	1	125	125	-10	2	5	239	187	0	3	18	70	59
-3	2	17	66	70	4	2	36	63	46	6	2	5	67	96	-8	2	2	100	93	-10	2	7	50	-66	0	3	19	48	-58
3	2	18	48	-46	-4	2	36	86	78	6	2	6	184	191	-8	2	3	92	106	-10	2	10	240	209	0	3	20	25	9
-3	2	19	60	-58	4	2	37	58	-50	6	2	7	225	-238	8	2	4	203	-183	-10	2	13	107	105	0	3	23	69	-68
3	2	20	50	62	-4	2	37	76	66	-6	2	7	59	-63	-8	2	4	120	129	10	2	20	92	77	0	3	24	55	-48
3	2	21	36	-44	-4	2	38	117	-102	6	2	8	188	202	8	2	5	93	-65	10	2	21	95	-99	0	3	25	106	95
3	2	22	104	106	5	2	0	51	31	6	2	9	115	140	8	2	6	204	-187	10	2	22	82	89	0	3	26	24	13
-3	2	22	74	76	5	2	1	89	-86	-6	2	9	69	-72	-8	2	6	152	-165	10	2	23	100	98	0	3	30	51	-58
-3	2	24	53	-53	-5	2	1	98	93	-6	2	10	93	-86	-8	2	8	164	-179	-11	2	4	56	59	0	4	0	34	-25
3	2	27	67	72	5	2	3	87	68	6	2	12	114	-133	-8	2	9	162	-144	-11	2	6	64	-28	0	4	1	30	-27
3	2	30	74	82	5	2	4	60	-69	-6	2	14	63	-50	8	2	10	153	145	-11	2	7	55	-69	0	4	2	76	67
3	2	31	63	-79	-5	2	4	146	120	6	2	15	186	-216	8	2	11	184	188	-11	2	8	54	38	0	4	3	34	24
3	2	32	80	88	5	2	5	81	-83	-6	2	15	64	58	-8	2	11	85	77	11	2	9	92	-75	0	4	4	17	-4
3	2	33	49	-74	-5	2	5	96	101	-6	2	16	95	-86	-8	2	12	146	147	-11	2	15	90	-84	0	4	5	27	-25
3	2	34	57	65	5	2	6	108	-113	-6	2	17	141	143	8	2	13	148	-127	-11	2	18	54	-63	0	4	6	24	-19
3	2	36	85	69	-5	2	6	302	-278	-6	2	20	66	-70	8	2	15	76	74	12	2	6	85	-103	0	4	7	34	-32
3	2	38	95	-86	-5	2	7	148	151	-6	2	21	54	-55	-8	2	15	123	-130	12	2	8	112	130	0	4	8	24	-16
-4	2	1	137	-128	5	2	8	102	123	-6	2	22	115	101	8	2	16	53	35	12	2	12	78	-76	0	4	9	37	-38
-4	2	2	148	125	5	2	9	64	-68	-6	2	23	111	-110	8	2	17	106	94	12	2	14	68	-63	0	4	11	29	15
4	2	3	70	-56	-5	2	9	130	114	-6	2	25	267	244	8	2	20	81	66	0	3	5	111	111	0	4	15	36	-39
-4	2	3	49	-39	5	2	10	92	-102	-6	2	26	122	115	-8	2	21	71	-89	0	3	6	77	80	0	4	17	25	2
4	2	4	74	54	5	2	11	74	-74	-6	2	27	114	-94	8	2	24	104	-84	0	3	11	79	-67	0	4	18	28	-35

by Van der Helm (1961*a*). A composite projection of the electron density distribution, which shows the deviation of the molecule from planarity, is shown in Fig. 1.

Three-dimensional refinement

Refinement was carried out by means of differential synthesis, calculated with a program written for the IBM 1620 (Damiani *et al.*, 1963), which uses output data of Van der Helm's structure factors program as input data (Van der Helm, 1961*b*). Scattering factors of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) were used for carbon and nitrogen atoms and that of McWeeny (1951) for hydrogen atoms. During the first three cycles an overall isotropic temperature factor was used and only the positional parameters of the carbon and nitrogen atoms were adjusted. After these calculations R had fallen to 0·20. During the next three cycles individual anisotropic temperature factors were assigned to the C and N atoms by comparing observed and calculated curvatures. R dropped to 0·13.

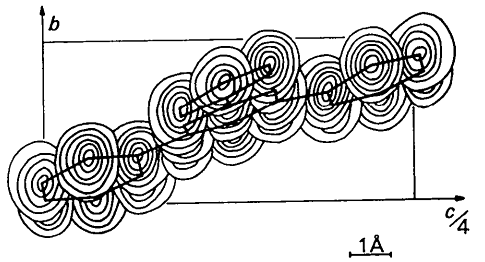

Fig. 1. Composite projection of the electron density distribution. Contours are at intervals of 1 e.Å^{-3}, beginning with the 1 e.Å^{-3} contour.

At this stage the hydrogen atoms were included at calculated positions, assuming C–H = 1·08 Å, with the same isotropic temperature factors of 4·0 Å^2. In the two final cycles of calculations all parameters, except the coordinates and the isotropic temperature factors of the hydrogen atoms, were simultaneously adjusted until the average shift in the atomic coordinates, in terms of their standard deviations, was less than 0·5 σ.

The final observed and calculated structure factors are given in Table 1; for these values R is 0·114. The final atomic parameters with their estimated standard deviations (Cruickshank, 1949) are given in Table 2. The lower accuracy of the y coordinates must be ascribed to the lack of reflexions of layer lines with $K > 3$. Furthermore the omission of the reflexions with $K > 3$ does not allow one to attach significance to the numerical values of anisotropic thermal parameters, listed in Table 3, and thus these must be only considered as parameters which improve the agreement between observed and calculated structure factors. On the other hand no corrections could be quantitatively made to the bond lengths for the apparent shortening due to thermal oscillations using the rigid-body approximations because of the non-planarity of the molecule. In fact some independent oscillation of the phenyl ring about the bonds connecting them to the triazine ring could be a significant feature of the thermal motion.

The values of observed and calculated electron-density peaks and curvatures are listed in Table 4. The estimated standard deviation of electron densities and its slopes are $\sigma(\varrho) = 0{\cdot}11$ e.Å^{-3}; $\sigma(A_h) = 0{\cdot}30$ e.Å^{-4}; $\sigma(A_k) = 0{\cdot}20$ e.Å^{-4}; $\sigma(A_l) = 0{\cdot}24$ e.Å^{-4}. The intramolecular distances and angles with their standard deviations are given in Table 5 and shown in Fig. 2. A view of the structure, showing the arrangement of the molec-

Table 2. *Final fractional atomic coordinates and their standard deviations* (Å)

	x/a	y/b	z/c	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
C(1)	−0·1725	0·6726	0·1911	0·0043	0·0065	0·0036
C(2)	−0·1157	0·8267	0·2214	0·0051	0·0074	0·0044
C(3)	−0·1764	0·8794	0·2544	0·0056	0·0078	0·0043
C(4)	−0·2983	0·7825	0·2570	0·0051	0·0081	0·0044
C(5)	−0·3555	0·6305	0·2272	0·0053	0·0077	0·0047
C(6)	−0·2955	0·5713	0·1941	0·0045	0·0073	0·0041
C(7)	−0·1704	0·2790	0·0637	0·0047	0·0066	0·0040
C(8)	−0·2926	0·1638	0·0663	0·0049	0·0081	0·0046
C(9)	−0·3520	0·0435	0·0349	0·0058	0·0082	0·0052
C(10)	−0·2953	0·0339	0·0010	0·0056	0·0084	0·0046
C(11)	−0·1737	0·1412	−0·0017	0·0059	0·0088	0·0048
C(12)	−0·1132	0·2611	0·0296	0·0053	0·0078	0·0046
C(13)	0·2039	0·6374	0·1235	0·0046	0·0064	0·0034
C(14)	0·2679	0·5201	0·0925	0·0050	0·0070	0·0040
C(15)	0·3948	0·5612	0·0920	0·0051	0·0087	0·0045
C(16)	0·4573	0·7120	0·1216	0·0058	0·0084	0·0050
C(17)	0·3930	0·8337	0·1524	0·0056	0·0079	0·0044
C(18)	0·2657	0·7919	0·1535	0·0049	0·0076	0·0043
C(19)	0·0694	0·5875	0·1247	0·0048	0·0068	0·0047
C(20)	−0·1065	0·4094	0·0972	0·0044	0·0068	0·0039
C(21)	−0·1073	0·6001	0·1565	0·0044	0·0069	0·0040
N(1)	0·0151	0·4634	0·0945	0·0037	0·0052	0·0030
N(2)	−0·1698	0·4743	0·1276	0·0039	0·0062	0·0033
N(3)	0·0149	0·6626	0·1564	0·0037	0·0057	0·0030

ules in the crystal is shown in Fig. 3. Intermolecular contacts less than 3·8 Å are given in Table 6.

Discussion

The geometry of the molecule, which represents the most interesting feature of the structure, was analysed by calculating the equations of the best planes passing through the atoms of the four molecular rings. The least-squares planes, calculated according to Schomaker, Waser, Marsh & Bergman (1959) with the aid of a program written for an IBM 1620 computer (Damiani *et al.*, 1962), are given in Table 7 together with the distances of the individual atoms from these planes. The best planes were determined with the same weight assigned to all atoms.

Table 3. *Final temperature parameters*

Temperature factors are given in the form exp $[-(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{13}hl)]$.

	b_{11}	b_{22}	b_{33}	b_{13}
C(1)	0·0038	0·0880	0·0005	0·0001
C(2)	0·0063	0·0860	0·0006	−0·0001
C(3)	0·0050	0·0900	0·0006	—
C(4)	0·0044	0·0960	0·0006	−0·0001
C(5)	0·0060	0·0887	0·0007	0·0001
C(6)	0·0048	0·0950	0·0006	−0·0001
C(7)	0·0037	0·0830	0·0006	—
C(8)	0·0043	0·0875	0·0007	−0·0001
C(9)	0·0071	0·0870	0·0008	0·0001
C(10)	0·0056	0·0900	0·0006	−0·0001
C(11)	0·0065	0·0900	0·0006	0·0001
C(12)	0·0044	0·0900	0·0006	—
C(13)	0·0041	0·0875	0·0004	—
C(14)	0·0034	0·0880	0·0006	—
C(15)	0·0045	0·0980	0·0007	−0·0001
C(16)	0·0056	0·0930	0·0008	—
C(17)	0·0044	0·0900	0·0007	0·0001
C(18)	0·0043	0·0880	0·0007	0·0001
C(19)	0·0044	0·0890	0·0005	0·0001
C(20)	0·0034	0·0870	0·0006	—
C(21)	0·0046	0·0880	0·0005	0·0001
N(1)	0·0046	0·0900	0·0005	—
N(2)	0·0044	0·0880	0·0005	−0·0001
N(3)	0·0046	0·0870	0·0005	−0·0001

The triazine ring and each of the three phenyl rings are almost exactly planar, but they are not coplanar. In fact the planes passing through the atoms of the phenyl groups attached to C(19), C(20) and C(21) are tilted with respect to the plane of the triazine ring at angles of 7·6°, 10·9° and 6·9° respectively, the sense of twist of the first two phenyl groups being opposite to that of the third one. As a further distortion the C(21)–C(1), C(7)–C(20) and C(19)–C(13) bonds are slightly moved out of the triazine plane through −0·7°, 1·5° and −2·2° respectively. In so far as coplanarity is a measure of conjugation it would appear that the phenyl groups are not completely conjugated with the triazine ring. Furthermore the great length of the C(21)–C(1), C(7)–C(20) and C(19)–C(13) bonds provide additional support for the conclusion that the conjugation between the rings is inhibited to some extent.

It is interesting to note that Farag (1954) has found that 1,3,5-triphenylbenzene is not planar in the solid state, the three phenyl groups being tilted with respect to the central ring through angles of 24°, 27° and 34° which are smaller than the average twist angle of 46° found in the vapour phase by means of electron diffraction methods (Bastianssen & Hassel, 1952). The phenyl groups are not twisted in the same sense and the average length of the bonds connecting them to the central ring is 1·50 Å.

Both *s*-triphenyltriazine and 1,3,5-triphenylbenzene in the crystal state lack a ternary symmetry axis perpendicular to the central ring. This may be explained by assuming that the gain in stability of the crystal due

Table 4. *Peak heights and curvatures*

Values in parentheses are from F_c differential synthesis

	ϱ (e.Å^{-3}) obs. calc.	$-A_{hh}$ (e.Å^{-5}) obs. calc.	$-A_{kk}$ (e.Å^{-5}) obs. calc.	$-A_{ll}$ (e.Å^{-5}) obs. calc.	A_{hk} (e.Å^{-5}) obs. calc.	A_{hl} (e.Å^{-5}) obs. calc.	A_{kl} (e.Å^{-5}) obs. calc.
C(1)	7·41	70·0	30·1	67·1	−2·8	0·0	−2·1
	(7·50)	(70·7)	(30·3)	(67·2)	(−1·9)	(−2·6)	(−1·3)
C(2)	6·71	58·8	26·7	55·1	−1·4	2·0	0·5
	(6·67)	(59·3)	(27·1)	(55·1)	(−1·1)	(0·2)	(0·0)
C(3)	6·47	53·7	25·2	56·8	−2·2	0·1	−0·8
	(6·56)	(56·1)	(26·0)	(57·1)	(−2·6)	(−0·8)	(−0·7)
C(4)	6·51	58·5	24·4	55·4	−3·5	4·5	−0·1
	(6·64)	(59·5)	(25·3)	(56·3)	(−3·3)	(0·7)	(0·0)
C(5)	6·40	55·9	25·4	51·1	−1·1	4·0	−0·7
	(6·44)	(54·1)	(25·9)	(51·7)	(−0·7)	(2·2)	(−0·5)
C(6)	6·95	65·9	27·1	58·8	−0·2	1·4	−2·7
	(6·94)	(64·7)	(27·7)	(58·5)	(−1·1)	(−0·3)	(−2·2)
C(7)	7·26	63·2	30·0	60·7	−1·9	1·0	−0·9
	(7·21)	(64·0)	(29·8)	(60·9)	(−1·8)	(0·1)	(−0·8)
C(8)	6·69	60·4	24·3	52·8	1·0	1·5	−0·4
	(6·68)	(61·0)	(24·9)	(53·2)	(0·6)	(−0·7)	(−0·3)
C(9)	6·20	51·3	23·9	46·2	−1·9	−0·6	0·4
	(6·14)	(49·7)	(24·5)	(46·3)	(−2·9)	(−0·5)	(−0·3)
C(10)	6·32	53·7	23·4	52·4	1·0	−1·3	1·0
	(6·40)	(54·6)	(24·0)	(52·9)	(0·8)	(−0·5)	(0·0)
C(11)	6·24	50·3	22·4	50·5	−1·8	3·6	−0·1
	(6·22)	(49·6)	(22·9)	(50·2)	(−1·3)	(2·8)	(0·0)
C(12)	6·63	55·8	25·2	53·2	1·4	0·4	−0·3
	(6·58)	(57·3)	(25·6)	(53·3)	(1·9)	(−0·4)	(−0·1)
C(13)	7·41	64·3	30·7	70·6	1·5	3·2	−3·3
	(7·48)	(62·7)	(31·0)	(70·7)	(0·7)	(2·1)	(−2·3)
C(14)	6·79	59·2	28·0	60·1	0·4	1·2	−2·0
	(6·97)	(59·8)	(28·8)	(60·8)	(−1·0)	(−0·3)	(−1·8)
C(15)	6·34	58·2	22·7	53·4	0·0	3·3	−1·1
	(6·58)	(58·6)	(24·3)	(54·3)	(−0·2)	(1·2)	(−0·5)
C(16)	6·14	51·8	23·4	48·0	3·3	−0·3	−0·9
	(6·24)	(53·3)	(24·5)	(49·1)	(1·5)	(−2·1)	(−0·5)
C(17)	6·47	53·1	24·8	54·5	2·9	−0·4	−2·4
	(6·57)	(53·8)	(25·8)	(55·3)	(1·5)	(−0·3)	(−2·4)
C(18)	6·62	61·3	25·8	56·6	0·5	−1·9	−2·9
	(6·70)	(61·9)	(26·5)	(56·8)	(0·0)	(−3·3)	(−2·5)
C(19)	7·22	61·9	28·9	66·1	−1·2	−1·7	−2·1
	(7·17)	(60·6)	(29·1)	(66·6)	(−2·1)	(−2·7)	(−1·2)
C(20)	7·18	67·4	29·1	62·2	−0·7	0·5	−2·6
	(7·19)	(67·1)	(29·5)	(61·8)	(−1·4)	(−0·4)	(−2·3)
C(21)	7·14	67·3	28·7	61·3	−1·6	−3·9	−2·3
	(7·07)	(66·0)	(28·7)	(60·2)	(−1·6)	(−5·6)	(−1·6)
N(1)	9·07	81·5	38·0	79·9	−0·6	0·0	−2·1
	(8·97)	(78·9)	(38·3)	(79·8)	(−1·1)	(−2·5)	(−2·3)
N(2)	8·50	75·9	31·5	72·5	0·7	2·0	−3·8
	(8·43)	(75·9)	(31·6)	(72·2)	(0·7)	(−1·1)	(−3·8)
N(3)	8·72	81·4	34·6	80·3	0·4	2·9	−0·9
	(8·73)	(78·9)	(34·8)	(79·2)	(−0·3)	(0·7)	(−0·8)

Table 5. *Intramolecular distances* (Å) *and angles* (°) *and standard deviations*

C(1)–C(2)	1·38$_3$	C(18)–C(13)	1·40$_1$	C(1)–C(2)–C(3)	121·5	N(1)–C(20)–N(2)	123·6
C(2)–C(3)	1·37$_8$	C(13)–C(19)	1·48$_5$	C(2)–C(3)–C(4)	119·2	N(2)–C(21)–N(3)	124·2
C(3)–C(4)	1·39$_0$	C(7)–C(20)	1·47$_4$	C(3)–C(4)–C(5)	119·8	N(1)–C(19)–N(3)	125·6
C(4)–C(5)	1·36$_8$	C(1)–C(21)	1·46$_5$	C(4)–C(5)–C(6)	121·7	C(19)–N(1)–C(20)	115·6
C(5)–C(6)	1·38$_2$	N(1)–C(19)	1·32$_1$	C(5)–C(6)–C(1)	118·8	C(20)–N(2)–C(21)	116·3
C(6)–C(1)	1·40$_8$	N(1)–C(20)	1·35$_1$	C(6)–C(1)–C(2)	118·9	C(21)–N(3)–C(19)	114·5
C(7)–C(8)	1·41$_5$	N(2)–C(20)	1·32$_2$	C(7)–C(8)–C(9)	119·5	C(2)–C(1)–C(21)	122·0
C(8)–C(9)	1·37$_6$	N(2)–C(21)	1·32$_9$	C(8)–C(9)–C(10)	121·3	C(6)–C(1)–C(21)	119·0
C(9)–C(10)	1·37$_1$	N(3)–C(21)	1·35$_9$	C(9)–C(10)–C(11)	119·5	C(1)–C(21)–N(2)	118·7
C(10)–C(11)	1·39$_9$	N(3)–C(19)	1·32$_2$	C(10)–C(11)–C(12)	119·6	C(1)–C(21)–N(3)	117·1
C(11)–C(12)	1·37$_8$	C(2)–N(3)	2·82$_0$	C(11)–C(12)–C(7)	121·3	C(8)–C(7)–C(20)	119·8
C(12)–C(7)	1·38$_1$	C(6)–N(2)	2·79$_1$	C(12)–C(7)–C(8)	118·7	C(12)–C(7)–C(20)	121·5
C(13)–C(14)	1·39$_7$	C(8)–N(2)	2·83$_6$	C(13)–C(14)–C(15)	118·6	C(7)–C(20)–N(1)	117·0
C(14)–C(15)	1·39$_8$	C(12)–N(1)	2·81$_7$	C(14)–C(15)–C(16)	121·3	C(7)–C(20)–N(2)	119·3
C(15)–C(16)	1·38$_7$	C(14)–N(1)	2·77$_6$	C(15)–C(16)–C(17)	120·0	C(14)–C(13)–C(19)	119·0
C(16)–C(17)	1·39$_9$	C(18)–N(3)	2·79$_3$	C(16)–C(17)–C(18)	119·4	C(18)–C(13)–C(19)	120·3
C(17)–C(18)	1·40$_3$			C(17)–C(18)–C(13)	120·0	C(13)–C(19)–N(1)	117·5
				C(18)–C(13)–C(14)	120·7	C(13)–C(19)–N(3)	116·9

The standard deviations of the bond lengths varied from 0·006 Å to 0·009 Å with an average value of 0·008$_1$ for the C–C bonds within the phenyl groups, 0·007$_0$ for the C–C bonds connecting the phenyl groups to the triazine ring and 0·006$_6$ for the C–N bonds. The average standard deviation of the bond angles was 0·5°.

to a presumably better packing, if the molecules had a higher symmetry, would not compensate the higher probability of a random conformation. The molecular structures of *s*-triphenyltriazine and 1,3,5-triphenylbenzene are therefore very similar and the deviation from planarity must be ascribed to steric inhibition of resonance for both the isosteric compounds. The smaller twist angles of the phenyl groups attached to the triazine ring are consistent with the presence of nitrogen atoms, which should imply weaker steric interactions of the *ortho* hydrogen atoms of the phenyl groups with the central ring. However any further comments on the values of twist angles experimentally determined in the solid state must be regarded as very tentative because intermolecular forces may represent an important role in determining the molecular geometry of these compounds. In fact biphenyl (Hargreaves & Hasan Rizvi, 1962) and 2,2′-bipyridyl (Bertinotti, Liquori & Pirisi, 1956; Merritt & Schroeder, 1956) are planar in the solid phase and there is strong experimental evidence that the two rings of the molecules are mutually inclined in solution and in the vapour phase. An angle of 42° between the planes of the rings is obtained by electron diffraction for biphenyl, where-

Table 6. *Intermolecular contacts less than* 3·8 Å

Roman numerals refer to the molecules:

I (*x*, 1+*y*, *z*)
II (−*x*, −*y*, −*z*)
III (−*x*, 1−*y*, −*z*)
IV (−*x*, ½+*y*, ½−*z*)
V (1+*x*, *y*, *z*)

C(1) ···· C(6)I	3·76 Å	C(17) ··· C(16)I	3·68 Å
C(2) ···· C(1)I	3·53	C(18) ··· C(13)I	3·54
C(2) ···· C(6)I	3·64	C(18) ··· C(14)I	3·59
C(3) ···· C(4)I	3·78	C(19) ··· N(1)I	3·64
C(3) ···· C(5)I	3·66	C(20) ··· C(7)I	3·67
C(3) ···· C(6)I	3·69	C(20) ··· C(8)I	3·74
C(4) ···· C(5)I	3·54	C(21) ··· N(2)I	3·63
C(7) ···· C(8)I	3·71	N(2) ···· C(8)I	3·72
C(7) ···· C(9)I	3·73	C(12) ··· C(11)II	3·66
C(8) ···· C(9)I	3·67	C(12) ··· C(12)III	3·77
C(11) ··· C(10)I	3·74	C(14) ··· C(10)III	3·79
C(12) ··· C(10)I	3·76	C(14) ··· C(11)III	3·65
C(12) ··· C(11)I	3·68	C(2) ···· C(2)IV	3·78
C(13) ··· C(14)I	3·70	C(3) ···· C(2)IV	3·74
C(16) ··· C(15)I	3·55	C(4)· ·· C(18)IV	3·79
C(17) ··· C(14)I	3·69	C(18) ··· C(4)IV	3·75
C(17) ··· C(15)I	3·57	C(16) ··· C(6)V	3·77

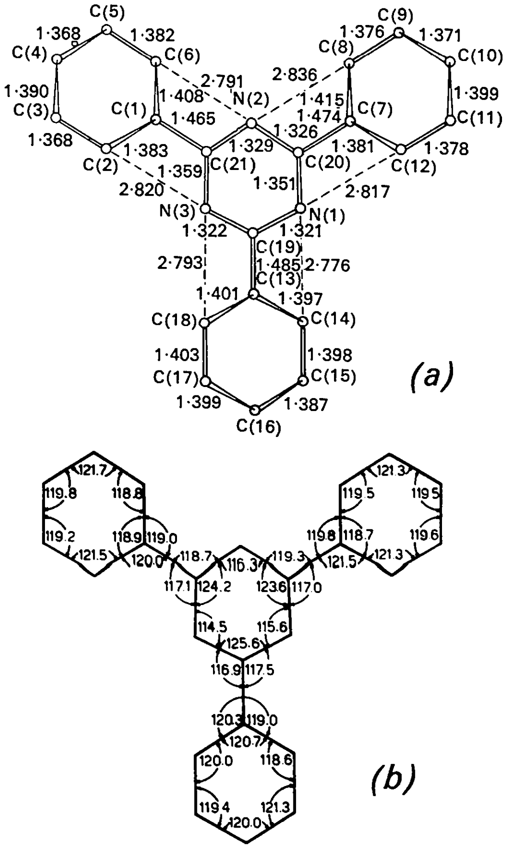

Fig. 2. (*a*) Intramolecular distances and (*b*) bond angles in s-triphenyltriazine.

as the results for 2,2′-bipyridyl are not conclusive (Almenningen & Bastianssen, 1958). Cumper, Ginnan & Vogel (1962) suggest a value of 18° for the twist angle in 2,2′-bipyridyl on the basis of electric dipole moment in benzene solution. Hargreaves & Hasan Rizvi (1962) attribute the observed differences in the molecular conformation of biphenyl in the vapour and solid state to crystal forces, assuming on the basis of the great length of the bond connecting the two phenyl groups (1·506 Å) that there is no conjugation between the rings. Therefore the planarity of the molecule in the crystal should be essentially determined by intermolecular contacts, which should produce a gain in energy greater than the energy due to steric repulsions between *ortho* hydrogen atoms. In the same way the planarity of 2,2′-bipyridyl in the crystal, where the molecule adopts a *trans* conformation, could be explained. Steric interactions between nitrogen and nearest CH groups of the other ring should be responsible, in this case, for the great length (1·50 Å) of the bond connecting the two rings. Similar intramolecular repulsions are present in *s*-triphenyltriazine with the exception that in this case each nitrogen atom interacts with two CH groups (from two phenyl rings). The average length of the bonds connecting the phenyl groups to the triazine ring is 1·475 Å, very close to the value of 1·477 Å proposed by Dewar & Schmeising (1959), for an sp^2-sp^2 σ bond with no π bonding between two carbon atoms.

However; possible slight differences in hybridization do not account for the degree of conjugation of the rings on the basis of this bond length only. In any case, the molecular geometry of *s*-triphenyltriazine, as compared with 1,3,5-triphenylbenzene, clearly shows that the presence of nitrogen atoms in the central ring is unable to relieve the stress due to steric interactions. It must be noted, of course, that intramolecular contacts between non-bonded atoms are different in the two unstrained molecules because of the differences in molecular parameters of the central rings.

Inspection of intermolecular distances (Table 6) shows that the packing of the molecules is very effici-

Table 7. *Equations of the planes referred to the crystallographic axes for the molecule at* $(-x, -\frac{1}{2}+y, \frac{1}{2}-z)$ *and distances of atoms from the planes*

Deviations from the plane through the triazine ring having equation:

$$0{\cdot}1704x+0{\cdot}9290y+0{\cdot}3265z=4{\cdot}5823$$

N(1)	0·001 Å	C(1)	−0·019 Å	C(7)	0·038 Å	C(13)	−0.058 Å
N(2)	−0·001	C(2)	0·080	C(8)	−0·183	C(14)	−0·241
N(3)	0·001	C(3)	−0·000	C(9)	−0·142	C(15)	−0·322
C(19)	−0·002	C(4)	−0·157	C(10)	0·114	C(16)	−0·237
C(20)	0·000	C(5)	−0·253	C(11)	0·309	C(17)	−0·036
C(21)	0·001	C(6)	−0·193	C(12)	0·265	C(18)	−0·037

Deviations from the plane through the phenyl group C(1) ··· C(6) having equation:

$$0{\cdot}2873x+0{\cdot}8983y+0{\cdot}3293z=4{\cdot}7932$$

C(1)	0·000 Å	C(3)	−0·008 Å	C(5)	0·002 Å
C(2)	0·006	C(4)	0·004	C(6)	−0·004

Deviations from the plane through the phenyl group C(7) ··· C(12) having equation:

$$0{\cdot}3164x+0{\cdot}9260y+0{\cdot}2025z=2{\cdot}9467$$

C(7)	0·009 Å	C(9)	−0·006 Å	C(11)	−0·003 Å
C(8)	−0·004	C(10)	0·009	C(12)	−0·006

Deviations from the plane through the phenyl group C(13) ··· C(18) having equation:

$$0{\cdot}1074x+0{\cdot}8922y+0{\cdot}4375z=6{\cdot}1436$$

C(13)	0·000 Å	C(15)	0·003 Å	C(17)	0·009 Å
C(14)	0·001	C(16)	−0·008	C(18)	−0·005

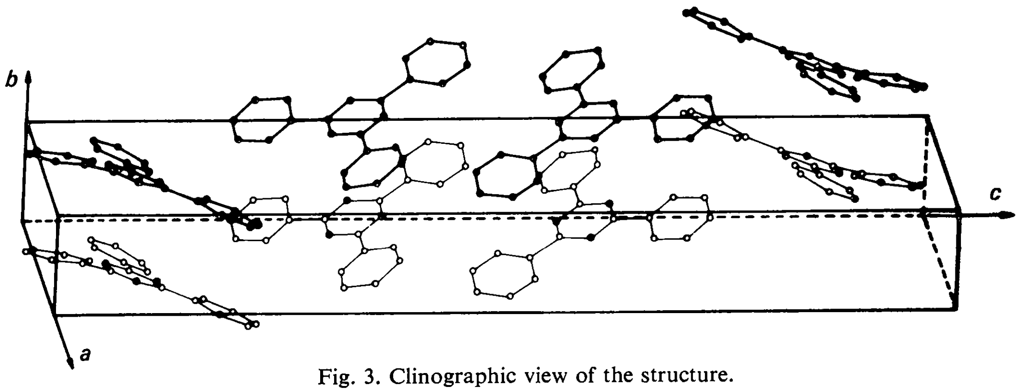

Fig. 3. Clinographic view of the structure.

ent. The shortest intermolecular distance is 3·53 Å and there is a large number of approaches less than 3·80 Å between C atoms of the phenyl rings. This suggests that intermolecular forces cannot be neglected when the extent of the deviation from planarity is considered. As it can be seen from Table 5 and Fig. 3, no significant deviation from the regularity of the phenyl groups can be deduced from the values of the bond angles and lengths.

The average bond length and angle within the phenyl groups are 1·390 Å and 120·0° respectively. The largest deviations from the average bond length are 0·022 Å and 0·019 Å for C(4)–C(5) and C(9)–C(10) respectively. These bonds, however, are at the perimeter of the molecule where the greatest errors caused by rigid body thermal motion should be expected.

The average values of 115·5° and 124·5° for the C–N–C and N–C–N bond angles within the triazine ring are 2·3° larger and 2·3° smaller respectively than the values found by Wheatley (1955) in *s*-triazine. The smallest value of the C–N–C angle further confirms the theoretical prediction made by Hameka & Liquori (1956) on the effect of sp^2 hybridization of the lone-pair electrons of the nitrogen atom on the bond angle. The lengths of C(19)–N(1), C(19)–N(3), C(20)–N(2) and C(21)–N(2) are very close to the value of 1·319 Å observed in non-substituted *s*-triazine, whereas the lengths of 1·351 Å and 1·359 Å of the C(20)–N(1) and C(21)–N(3) bonds are significantly larger, as far as the standard deviations are considered.

The safest conclusion which may be drawn from the above results is that the intramolecular steric repulsions in *s*-triphenyltriazine are responsible for the non-planarity of the molecule and that the extent of distortion allowed by a decreased rigidity of the bonds connecting the phenyl groups to the triazine ring might be influenced by intermolecular contacts.

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