392. *Topochemistry. Part X.*[1] *The Crystal and Molecular Structures of 2-Chloro-N-salicylideneaniline.*

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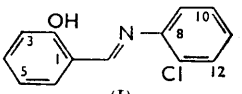
The structure of 2-chloro-*N*-salicylideneaniline has been determined from three-dimensional data. The co-ordinates of carbon, nitrogen, oxygen, and chlorine have been located by an anisotropic least-squares refinement to an accuracy of at least 0·003 Å. The positional and isotropic temperature parameters of the hydrogen atoms have also been obtained. The electron-density distribution in the O · · · N region has been determined by three-dimensional difference syntheses; the hydrogen atom identified with the electron-density peak in this region was included in the final stages of the least-squares refinement.

Molecular shape, packing arrangement, and bond lengths of 2-chloro-*N*-salicylideneaniline (2-chloroanil) and of *N*-5-chlorosalicylideneaniline (5′-chloroanil) (Part IX) are compared and discussed.

THE detailed analysis of the crystal structure of (photochromic) 2-chloro-*N*-salicylideneaniline (I) * was undertaken as part of a research programme on the relation between crystal structure and solid-state thermochromy and photochromy (see preceding Papers). The aims of this analysis are set out in Part IX [1] in which we describe the crystal structure of (thermochromic) *N*-5-chlorosalicylideneaniline.



(I)

EXPERIMENTAL

2-Chloro-*N*-salicylideneaniline, $C_{13}H_{10}ClNO$, *M* 231·7, crystallises from methylcyclohexane in pale yellow orthorhombic needles elongated along [001] and showing {110}. The cell dimensions were determined from high-order reflections recorded on a General Electric goniostat: $a = 13{\cdot}528$, $b = 12{\cdot}185$, $c = 6{\cdot}871$ Å; $\sigma(a) = 0{\cdot}0010$, $\sigma(b) = 0{\cdot}0008$, $\sigma(c) = 0{\cdot}0006$ Å. Absences: $h00$ for h odd, $0k0$ for k odd, $00l$ for l odd. *Space group*: $P2_12_12_1$. d(calc.) for $n = 4$, 1·359 g./cm.^{3}; $\mu = 30{\cdot}0$ cm.$^{-1}$; $F(000) = 480$.

TABLE 1.

Atomic co-ordinates (Å).

Atom	*x*	*y*	*z*	Atom	*x*	*y*	*z*
C_1	9·780	−1·468	4·224	N	7·537	−0·726	4·590
C_2	9·565	−1·866	2·909	O	8·339	−1·739	2·323
C_3	10·595	−2·435	2·163	Cl	5·831	1·498	3·581
C_4	11·843	−2·593	2·749				
C_5	12·091	−2·179	4·030	H_3	10·408	−2·716	1·144
C_6	11·062	−1·618	4·768	H_4	12·695	−2·984	2·230
				H_5	12·926	−2·417	4·584
C_7	8·722	−0·921	5·055	H_6	11·262	−1·262	5·811
C_8	6·510	−0·310	5·478	H_7	8·991	−0·733	6·088
C_9	6·324	−0·930	6·702	H_9	6·935	−1·679	6·981
C_{10}	5·303	−0·544	7·529	H_{10}	5·120	−0·994	8·405
C_{11}	4·456	0·484	7·173	H_{11}	3·804	0·857	7·750
C_{12}	4·614	1·106	5·956	H_{12}	4·006	1·853	5·662
C_{13}	5·640	0·697	5·110	H_0	7·708	−1·246	3·151

The zonal data $F(hk0)$ and $F(h0l)$ were collected from zero-level Weissenberg photographs and processed in the usual way. The set of three-dimensional reflections was recorded on the goniostat with nickel-filtered copper radiation and an argon-filled counter from a crystal shaped to linear dimensions 0·15 × 0·15 × 0·15 mm.; absorption corrections were considered unnecessary. We refer to Part V [2] for details of our treatment of data, their reduction of $F(hkl)$,

* The numbering shown in (I) is that used in crystallographic descriptions and in bond dimensions.

[1] Part IX, preceding paper.

and calculation of associated weights $w(hkl)$. Since the tube output was heavily contaminated with iron radiation all reflections with indices h, k, and l divisible by five were given zero weight.

Solution of the Structure.—The Patterson projection $P(xy)$ was insufficiently resolved to enable us to locate the chlorine atom, let alone the lighter atoms, with sufficient accuracy for a trial structure. The heavy-atom co-ordinates were established from $P(xy)$ and $P(xz)$ of the isomorphous bromo-derivative ($a = 13{\cdot}6$, $b = 12{\cdot}3$, $c = 7{\cdot}19$ Å; space group $P2_12_12_1$); the two sets of intensity data were put on an approximately absolute scale and the signs of a number of

TABLE 2.

Thermal parameters (Å²).

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
C_1	0·0570	0·0437	0·0579	−0·0018	0·0012	0·0002
C_2	0·0669	0·0481	0·0611	−0·0033	0·0028	0·0053
C_3	0·0872	0·0565	0·0642	−0·0052	0·0016	0·0203
C_4	0·0698	0·0558	0·0901	−0·0022	−0·0001	0·0273
C_5	0·0589	0·0637	0·0920	−0·0021	−0·0009	0·0073
C_6	0·0589	0·0556	0·0764	−0·0077	−0·0013	−0·0025
C_7	0·0552	0·0483	0·0621	−0·0046	−0·0012	−0·0035
C_8	0·0516	0·0468	0·0568	0·0011	−0·0086	−0·0059
C_9	0·0654	0·0538	0·0575	0·0041	0·0011	−0·0024
C_{10}	0·0783	0·0655	0·0647	0·0032	−0·0011	0·0101
C_{11}	0·0678	0·0671	0·0735	0·0053	−0·0059	0·0112
C_{12}	0·0615	0·0553	0·0761	0·0053	−0·0074	−0·0086
C_{13}	0·0614	0·0466	0·0511	−0·0040	−0·0031	−0·0101
N	0·0564	0·0510	0·0556	0·0015	−0·0069	−0·0023
O	0·0757	0·0935	0·0592	0·0111	−0·0111	−0·0119
Cl	0·0960	0·0736	0·0597	0·0081	0·0115	−0·0084

Atom	U
H_3	0·0403
H_4	0·0666
H_5	0·0409
H_6	0·0387
H_7	0·0354
H_9	0·0633
H_{10}	0·0473
H_{11}	0·0507
H_{12}	0·0385
H_0	0·1042

TABLE 3.

Standard deviations (Å) of atomic co-ordinates.

Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
C_1	0·0026	0·0027	0·0031	N	0·0022	0·0022	0·0024
C_2	0·0028	0·0028	0·0032	O	0·0020	0·0020	0·0020
C_3	0·0033	0·0031	0·0033	Cl	0·0009	0·0009	0·0009
C_4	0·0031	0·0029	0·0036	H_3	0·026	0·027	0·029
C_5	0·0030	0·0032	0·0036	H_4	0·031	0·032	0·031
C_6	0·0029	0·0030	0·0032	H_5	0·025	0·027	0·028
C_7	0·0027	0·0029	0·0031	H_6	0·025	0·028	0·028
C_8	0·0027	0·0026	0·0029	H_7	0·025	0·027	0·029
C_9	0·0029	0·0028	0·0032	H_9	0·027	0·031	0·032
C_{10}	0·0034	0·0032	0·0034	H_{10}	0·028	0·030	0·028
C_{11}	0·0031	0·0032	0·0036	H_{11}	0·027	0·029	0·034
C_{12}	0·0029	0·0030	0·0035	H_{12}	0·025	0·029	0·027
C_{13}	0·0029	0·0026	0·0028	H_0	0·033	0·035	0·040

TABLE 4.

Standard deviations (Å²) of thermal parameters.

Atom	$\sigma(U_{11})$	$\sigma(U_{22})$	$\sigma(U_{33})$	$\sigma(U_{12})$	$\sigma(U_{23})$	$\sigma(U_{13})$
C_1	0·0015	0·0013	0·0017	0·0014	0·0015	0·0015
C_2	0·0017	0·0014	0·0019	0·0014	0·0015	0·0017
C_3	0·0020	0·0016	0·0019	0·0017	0·0017	0·0019
C_4	0·0018	0·0017	0·0022	0·0016	0·0019	0·0019
C_5	0·0017	0·0017	0·0023	0·0016	0·0020	0·0020
C_6	0·0016	0·0016	0·0021	0·0015	0·0019	0·0018
C_7	0·0015	0·0013	0·0019	0·0013	0·0015	0·0016
C_8	0·0014	0·0013	0·0018	0·0013	0·0015	0·0015
C_9	0·0016	0·0014	0·0018	0·0015	0·0016	0·0017
C_{10}	0·0019	0·0017	0·0020	0·0018	0·0018	0·0020
C_{11}	0·0018	0·0018	0·0022	0·0016	0·0019	0·0019
C_{12}	0·0017	0·0016	0·0022	0·0015	0·0016	0·0018
C_{13}	0·0016	0·0013	0·0017	0·0014	0·0013	0·0015
N	0·0012	0·0012	0·0014	0·0012	0·0012	0·0013
O	0·0013	0·0015	0·0013	0·0014	0·0014	0·0012
Cl	0·0005	0·0004	0·0005	0·0005	0·0005	0·0005

Atom	$\sigma(U)$
H_3	0·0088
H_4	0·0117
H_5	0·0088
H_6	0·0088
H_7	0·0085
H_9	0·0099
H_{10}	0·0091
H_{11}	0·0095
H_{12}	0·0085
H_0	0·0147

reflections established by the usual method. Fourier projections were sufficiently detailed to permit least-squares refinement of the two zones of the chloro-compound to R($hk0$) = 0·093 and R($h0l$) = 0·112 [$F_{(\text{unobserved})}$ excluded; all hydrogens bonded to carbon were included on the basis of reasonable bond length (C–H = 1·0 Å) and angles; hydroxylic hydrogen was omitted; C,N,O,Cl treated anisotropically]. The resulting structure served as the basis for a three-

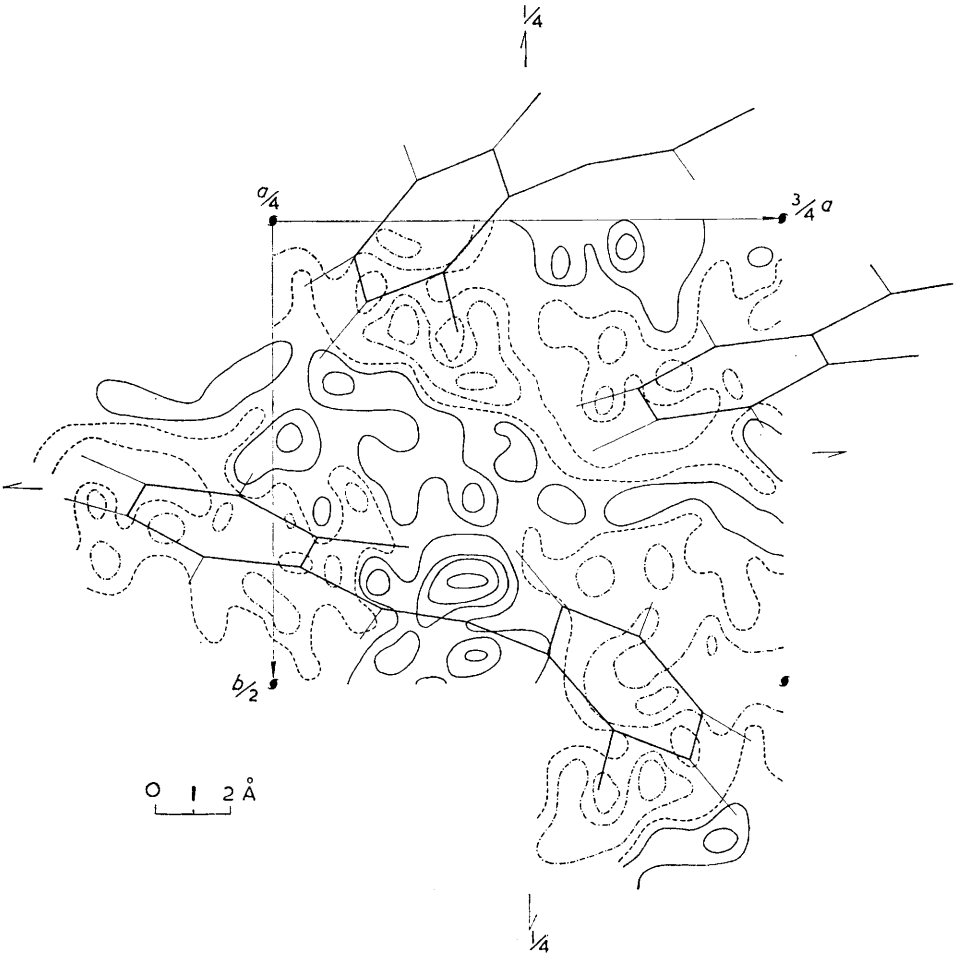


FIG. 1. 2-Chloro-*N*-salicylideneaniline; δ(xy) based on all atoms except hydroxyl hydrogen. Contour interval 0·1 e/Å²; zero contour – – – –, negative contours — · — · —.

dimensional refinement which proceeded by anisotropic cycles for all atoms, except the hydrogens which were held fixed until the heavy atoms had settled down; in further cycles the positional and isotropic thermal parameters of the hydrogens were also adjusted. For details of the least-squares procedure we refer to Part V.[2] The following scattering-factor curves were used: f_{Cl}, Dawson,[3] $f_{C,N,O}$ Berghuis *et al.*,[4] f_H, McWeeny.[5] No allowance was made for anomalous-dispersion effects of the chlorine atom.

To locate the hydrogen in the O · · · N region we computed the difference syntheses δ(xy)

[2] Part V, *J.*, 2030.
[3] Dawson, *Acta Cryst.*, 1960, **13**, 403.
[4] Berghuis, Haanappel, Potters, Loopstra, MacGillavry, and Veenendaal, *Acta Cryst.*, 1955, **8**, 478.
[5] McWeeny, *Acta Cryst.*, 1951, **4**, 513.

(Fig. 1) and $\delta(xz)$ both of which showed peaks of height 0·4 e/Å^2 in the O · · · N region. Three-dimensional difference syntheses (Fig. 2) in planes parallel to (001) were computed in the region corresponding to these peaks in the $\delta(xy)$ and $\delta(xz)$ maps. Reflections affected by iron contamination of the copper tube and those for which $|hF_o| > 2|F_c|$ were omitted from the difference syntheses; $\Delta F(230)$, corresponding to the strongest reflection (230) believed to suffer from secondary extinction, was also omitted. The three-dimensional plane syntheses showed

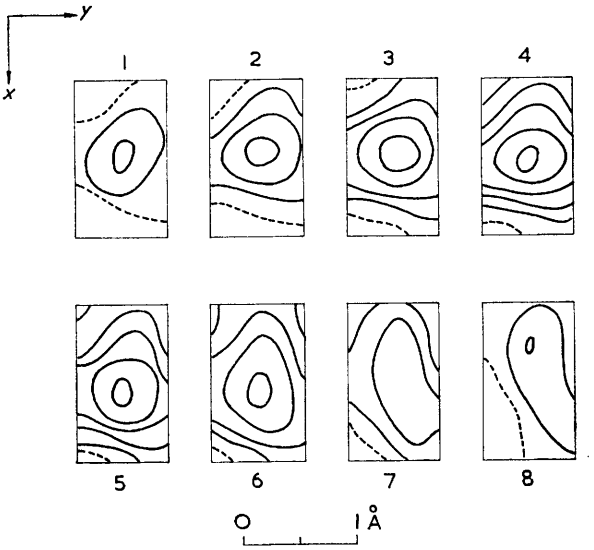


FIG. 2. 2-Chloro-*N*-salicylideneaniline; parallel sections perpendicular to [001] of $\delta(xyz)$ in the O · · · N region. Contour interval 0·05 e/Å^3; upper left corner of each section at $x = 0{\cdot}513$, $y = -0{\cdot}139$; first section at $z = 0{\cdot}375$. Distance between sections 0·2 Å; increasing z sections from 1 to 8.

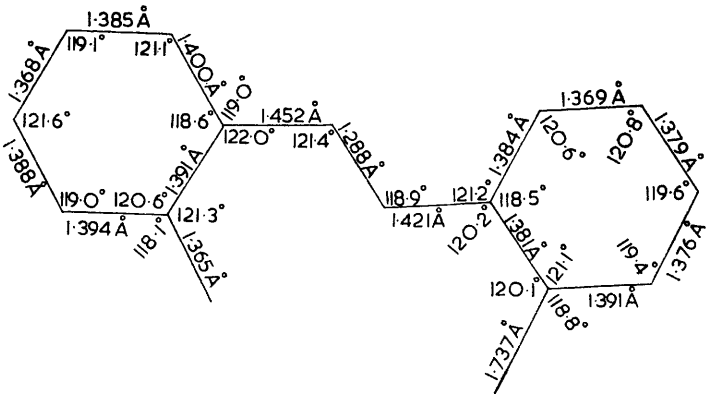


FIG. 3. 2-Chloro-*N*-salicylideneaniline; experimentally determined bond lengths and bond angles.

a peak of height 0·25 e/Å^3 at 1·25 Å from the oxygen, 1·45 Å from the nitrogen, and at 0·07 Å from the best plane defined by O,C_2,C_1,C_7,N. On the assumption that this peak might refer to the hydroxylic hydrogen, refinement of the structure was continued with this hydrogen included. The last cycle gave an O–H distance of 1·15 Å, a C_2OH angle of 103°, and deviation of 0·02 Å from the best plane of ring c (O, C_2,C_1,C_7,N).

Refinement was stopped when all parameter shifts had become less than $\frac{1}{10}$ their estimated standard deviations. The final agreement factor $r = \Sigma w(k^2F_o^2 - |F_c|^2)^2/\Sigma wk^4F_o^4$ was 0·006,

($R = \Sigma|kF_o - |F_c||/\Sigma kF_o$ was 0·046) for all reflections excluding those for which $|F_c| < |kF_{threshold}|$.

The positional and thermal parameters derived from the last refinement cycle, and their standard deviations, estimated according to Part V,[2] are listed in Tables 1—4. Bond lengths and angles are given in Fig. 3; Table 5 lists the e.s.d. of the bond lengths, while the C–H bond lengths and angles are given in Table 6. The best planes through rings A(C_{1-6}), B (C_{8-13}), and C (O, C_2, C_1, C_7,N) were computed according to Schomaker *et al.*; [6] (Table 7 lists their equations, as well as the distances of the substituents and ring atoms from these planes. Table 8 contains *hkl*, 100 kF_o, 100 A_c, 100 B_c, and 100 F_c. Reflections to which zero weight was attached are marked *; all unobserved reflections are marked $<kF_o$.

TABLE 5.

Standard deviation of bond lengths (Å).

Bond		Bond		Bond		Bond	
C_1–C_2	0·0040	C_7–N	0·0037	C_8–C_{13}	0·0039	C_7–H_7	0·027
C_2–C_3	0·0043	N–C_8	0·0035	C_{13}–Cl	0·0029	C_9–H_9	0·030
C_3–C_4	0·0045	C_8–C_9	0·0040	C_2–O	0·0035	C_{10}–H_{10}	0·029
C_4–C_5	0·0046	C_9–C_{10}	0·0045	C_3–H_3	0·027	C_{11}–H_{11}	0·030
C_5–C_6	0·0044	C_{10}–C_{11}	0·0047	C_4–H_4	0·032	C_{12}–H_{12}	0·027
C_6–C_1	0·0041	C_{11}–C_{12}	0·0045	C_5–H_5	0·027	O–H_0	0·036
C_1–C_7	0·0040	C_{12}–C_{13}	0·0042	C_6–H_6	0·027		

TABLE 6.

C–H Bond lengths and angles.

Bond	Bond length (Å)	Bond angles (°)			
C_3–H_3	1·073	C_2–C_3–H_3	119·1	C_4–C_3–H_3	121·8
C_4–H_4	1·072	C_3–C_4–H_4	123·5	C_5–C_4–H_4	114·8
C_5–H_5	1·030	C_4–C_5–H_5	125·5	C_6–C_5–H_5	114·1
C_6–H_6	1·120	C_5–C_6–H_6	119·5	C_1–C_6–H_6	119·4
C_7–H_7	1·084	C_1–C_7–H_7	115·5	N–C_7–H_7	123·1
C_9–H_9	1·006	C_8–C_9–H_9	119·8	C_{10}–C_9–H_9	119·6
C_{10}–H_{10}	1·002	C_9–C_{10}–H_{10}	122·6	C_{11}–C_{10}–H_{10}	116·6
C_{11}–H_{11}	0·947	C_{10}–C_{11}–H_{11}	124·0	C_{12}–C_{11}–H_{11}	116·1
C_{12}–H_{12}	1·008	C_{11}–C_{12}–H_{12}	121·6	C_{13}–C_{12}–H_{12}	119·1
O–H_0	1·152	C_2–O–H_0	102·9		

TABLE 7.

Equations of best planes.

		m_1	m_2	m_3	d
Ring A	$C_1 \cdots C_6$	3·5019	11·0594	−2·2708	−0·1857
Ring B	$C_8 \cdots C_{13}$	8·2478	8·1382	+2·9332	6·0936
Ring C	O, C_2, C_1, C_7, N	3·3961	11·1617	−2·1499	−0·2201

Equation of best plane: $m_1x + m_2y + m_3z - d = 0$, where *xyz* are fractional co-ordinates.

Deviations (Å) from best planes.

Atom	Ring A	Ring C	Atom	Ring B
C_1	−0·011	+0·009	C_8	+0·008
C_2	+0·007	+0·002	C_9	+0·002
C_3	+0·004		C_{10}	−0·010
C_4	−0·010		C_{11}	+0·008
C_5	+0·006		C_{12}	+0·001
C_6	+0·005		C_{13}	−0·009
C_7	−0·063	−0·016	N	−0·024
O	−0·002	−0·006	Cl	−0·010
N	−0·039	+0·011		

Comparison of the Structures of N-5-*Chloro- and* 2-*Chloro*-N-*salicylideneaniline*.—In the 2-chloroanil rings A and C lie on a common plane to within 1° of the normals to their respective best planes. The angle between ring A and the anil ring (B) of 51·5° is due to rotation of the

[6] Schomaker, Waser, Marsh, and Bergman, *Acta Cryst.*, 1959, **12**, 600.

latter around the C_8–N bond since the angle between the vectors C_9–C_{13} and C_2–C_6 corresponds to 51·1°. In addition, the deviations of N, C_8, centre of ring B, and of C_{11} from the plane of ring A linearly increase (by −0·039, −0·221, −0·411, and −0·592 Å) so that the molecule is bent into a V shape where the nitrogen is at the apex and the angle between the arms of the V is 7·5°. Rotation of the anil ring about C_8–N has led to a distance between (the *ortho*-hydrogen) H_9 and (the exocyclic hydrogen) H_7 of 2·43 Å corresponding to normal van der Waals contact.

In the 5′-chloroanil on the other hand the two rings A and B are parallel, both at room and

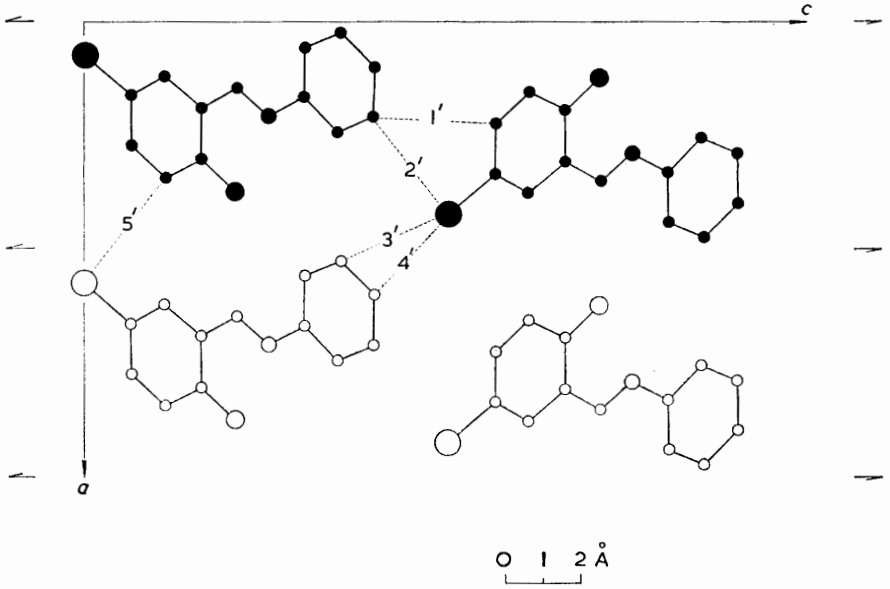


FIG. 4a. *N*-5-Chlorosalicylideneaniline; packing diagram seen along [010]. For contact distances see Table 11.

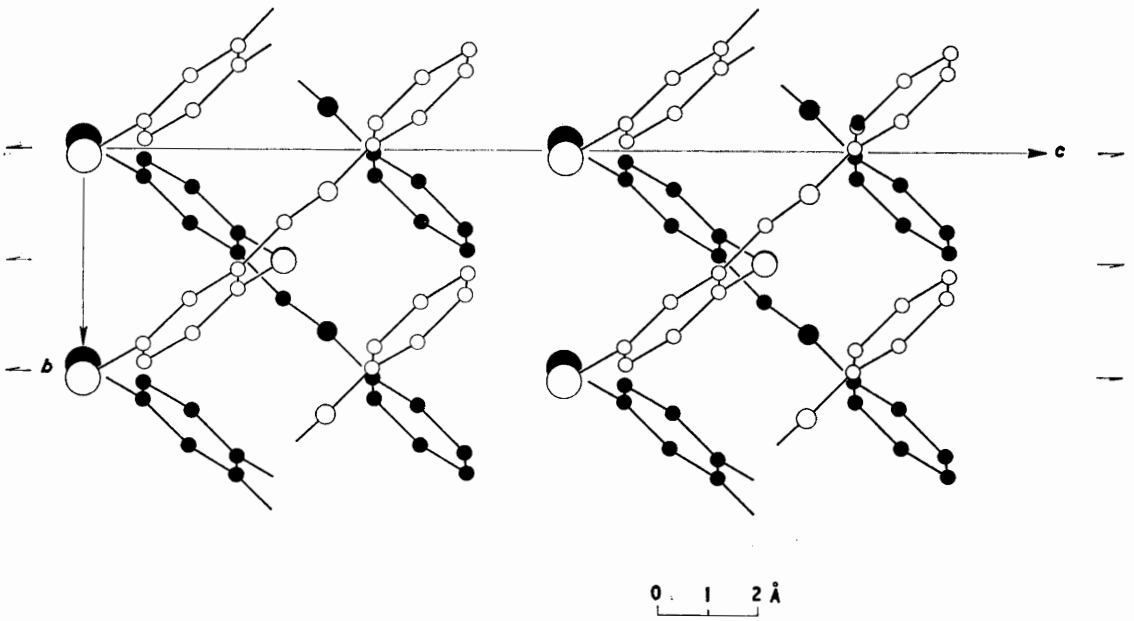


FIG. 4b. *N*-5-Chlorosalicylideneaniline; packing diagram seen along [100].

TABLE 8.

Structure factors.

h	k	l	$100kF_o$	$100A_c$	$100B_c$	$100F_c$
2	0	0	2371	2183	0	2183
4			5270	−5294	0	5294
6			2203	−2182	0	2182
8			1483	−1532	0	1532
10		*	746	165	0	165
12			369	−328	0	328
14			234	208	0	208
16			209	−106	0	106
1	1	0	1274	0	−991	991
2			3217	3093	0	3093
3			5780	0	6158	6158
4			1977	1948	0	1948
5			2329	0	2376	2376
6			1407	1381	0	1381
7			1390	0	1399	1399
8			486	−443	0	443
9			461	0	−413	413
10			1148	−1109	0	1109
11			712	0	−681	681
12			1291	−1241	0	1241
13			1148	0	1111	1111
14			202	73	0	73
15			461	0	421	421
16			293	238	0	238
17			150	0	135	135
0	2	0	5621	5766	0	5766
1			2060	0	−2255	2255
2			4926	4753	0	4753
3			1877	0	1845	1845
4		*	419	−173	0	173
5			1683	0	1741	1741
6			1567	1534	0	1534
7			1977	0	2041	2041
8			1055	−1037	0	1037
9			2346	0	2348	2348
10			872	−866	0	866
11			1592	0	−1561	1561
12			796	786	0	786
13			636	0	−598	598
14			<126	−10	0	10
15			<118	0	−46	46
16			202	−154	0	154
17			192	0	−163	163
1	3	0	8562	0	8846	8846
2			9501	10,226	0	10,226
3			1089	0	−1124	1124
4			1064	979	0	979
5			2354	0	−2389	2389
6			495	463	0	463
7			1315	0	−1334	1334
8			1089	−1089	0	1089
9			293	0	211	211
10			997	−950	0	950
11			2254	0	2226	2226
12			1809	−1768	0	1768
13			645	0	679	679
14			<126	15	0	15
15			<109	0	18	18
16			<168	95	0	95
17			168	0	−122	122
0	4	0	8478	−8690	0	8690
1			4817	0	4880	4880
2			880	825	0	825
3			1424	0	1455	1455
4			1257	1294	0	1294
5			478	0	−484	484
6			1641	1665	0	1665
7			495	0	465	465
8			1826	1754	0	1754
9			779	0	765	765
10			243	217	0	217
11			1165	0	−1178	1178
12			175	68	0	68
13			586	0	−580	580
14			369	−340	0	340
15			<109	0	24	24
16			<160	−24	0	24
1	5	0	1944	0	−1961	1961
2			946	−951	0	951
3			3191	0	−3246	3246
4			2028	−2045	0	2045
5			1441	0	−1397	1397
6			662	−684	0	684
7			737	0	740	740
8			1306	1267	0	1267
9			603	0	589	589
10		*	1893	−1729	0	1729
11			301	0	288	288
12			209	−250	0	250
13			<134	0	135	135
14			<118	118	0	118
15			<168	0	25	25
16			217	−164	0	164
0	6	0	1550	−1474	0	1474
1			2479	0	2509	2509
2			1190	−1164	0	1164
3			3267	0	3235	3235
4			788	759	0	759
5			704	0	−719	719
6			268	−312	0	312
7			444	0	−465	465
8			537	532	0	532
9			2028	0	−2052	2052
10			1416	1406	0	1406
11			352	0	347	347
12			343	−278	0	278
13			160	0	55	55
14			360	−269	0	269
15			377	0	238	238
16			202	125	0	125
1	7	0	737	0	−697	697
2			2035	−1954	0	1954
3			1382	0	1383	1383
4			1525	−1401	0	1401
5			1055	0	1055	1055
6			160	247	0	247
7			<134	0	87	87
8			670	664	0	664
9			411	0	438	438
10			687	−668	0	668
11			678	0	−701	701
12			<126	134	0	134
13			662	0	−649	649
14			469	−317	0	316
15			160	0	11	11
0	8	0	385	−334	0	334
1			1281	0	1265	1265
2			285	−290	0	290
3			511	0	−482	482
4			929	867	0	867
5			202	0	−166	166
6			343	−299	0	299
7			175	0	−39	39
8			662	−678	0	678
9			921	0	920	920
10			<134	171	0	171
11			<134	0	−54	54
12			243	129	0	129
13			<109	0	−57	57
14			175	160	0	160
1	9	0	310	0	−176	176
2			905	905	0	905
3			1232	0	1275	1275
4			754	730	0	730
5			746	0	711	711
6			788	734	0	734
7			377	0	366	366
8			1055	−1070	0	1070
9			251	0	−174	174
10			310	323	0	323
11			411	0	−463	463
12			<118	−152	0	152
13			192	0	−272	272
14			226	−247	0	247
0	10	0*	963	−904	0	904
1			1198	0	−1198	1198
2			427	−445	0	445
3			<134	0	70	70
4			175	279	0	279
5		*	486	0	257	257
6			285	243	0	243
7			503	0	439	439
8			461	481	0	481
9			1114	0	1160	1160
10		*	293	−218	0	218
11			168	0	204	204
12			<150	−20	0	20
13			143	0	59	59
1	11	0	175	0	102	102
2			569	−555	0	555
3			863	0	−841	841
4			594	529	0	529
5			436	0	−336	336
6			217	134	0	134
7			394	0	425	425
8			<126	−81	0	81
9			259	0	250	250
10			285	−286	0	286
11			185	0	143	143
12			202	−107	0	107
0	12	0	1340	−1368	0	1368
1			327	0	−440	440
2			<134	−77	0	77
3			461	0	460	460
4			<126	−5	0	4
5			168	0	202	202
6			670	684	0	684
7			<118	0	149	149
8			377	372	0	372
9			<160	0	60	60
10			<150	−196	0	196
11			175	0	252	252
1	13	0	285	0	−307	307
2			327	−342	0	342
3			695	0	−730	730
4			1114	−1020	0	1020
5			234	0	171	171
6			369	−369	0	369
7			<168	0	−23	23
8			259	163	0	163
9			150	0	135	135
0	14	0	343	358	0	358
1			569	0	577	577
2			143	−53	0	53
3			<109	0	119	119
4			<168	−95	0	95
5			<150	0	53	53
6			<143	135	0	135
7			251	0	−271	271
1	15	0	343	0	−411	411
2			168	−154	0	154
3			217	0	149	149
4			461	−506	0	506
1	0	1	4992	0	5274	5274
2			687	0	−590	590
3			2304	0	2294	2294
4			5186	0	5400	5400
5			1542	0	1525	1525
6			1055	0	−1012	1012
7			905	0	−892	892
8			1306	0	−1292	1292
9			855	0	−861	861
10			1399	0	−1383	1383
11			1106	0	−1166	1166
12			402	0	−432	432
13			1249	0	1228	1228
14			377	0	−374	374
15			175	0	190	190
16			243	0	179	179
17			293	0	−258	258
0	1	1	4206	0	4074	4074
1			762	−299	669	733
2			6024	−1220	−6113	6233
3			2706	2132	1653	2697
4			1977	−657	−1789	1906
5			1919	−1867	−149	1873
6			1039	−104	1111	1116
7			3694	−3406	1108	3582
8			1474	19	1493	1493
9			670	−271	−565	627
10			971	344	942	1003
11			980	−540	−889	1040
12			1249	−1096	−614	1256
13			662	557	254	613
14			453	−393	−192	437
15			636	613	26	613
16			150	−196	−93	217
17			101	61	−61	86
0	2	1	796	598	0	598
1			8143	7155	4230	8312
2			5420	73	−5523	5523
3			6752	6475	2049	6792
4			2572	−2366	−679	2462
5			4876	4786	−332	4797
6			1742	−1714	171	1722
7			914	−892	290	938
8			1030	829	−659	1059
9			1264	−986	−687	1202
10			762	701	−363	790
11			427	503	198	540
12			318	−21	−325	325
13			579	−591	220	631
14			160	94	−45	104
15			168	−55	17	58
16			234	−62	218	226
17			134	22	−112	114
0	3	1	3024	0	−3165	3164
1			6928	−3441	6272	7154
2			6652	3624	−5586	6657
3			2094	419	2107	2148

TABLE 8. (*Continued.*)

h	k	l	100kF_o	100A_c	100B_c	100F_c
4	3	1	545	−150	529	550
5			453	−287	−200	350
6			2555	−1241	2167	2498
7			1692	1672	160	1679
8			202	−99	80	127
9			520	346	−387	519
10			662	−697	−156	714
11			887	19	−866	867
12			343	284	203	349
13			552	−298	−434	527
14			411	−459	37	461
15			134	−71	156	171
16			243	−283	−84	295
0	4	1	3753	−3663	0	3663
1			3619	−2942	2030	3574
2			1609	743	−1418	1601
3			1441	1327	−368	1377
4			3913	−1558	−3764	4074
5			2673	2590	324	2610
6			1198	−907	−826	1227
7			594	492	381	622
8			335	−192	−158	249
9			670	441	589	736
10			1784	695	1659	1799
11			402	−85	394	404
12			720	750	131	762
13			579	−68	−573	577
14			369	−353	5	353
15			185	55	123	135
16			<109	−111	−51	122
0	5	1	478	0	−443	443
1			3511	−3220	1102	3403
2			1919	1021	1692	1976
3			2907	647	2843	2916
4			1207	−1195	−353	1246
5			1809	1838	−211	1850
6			234	−190	−209	283
7			1961	1597	−1120	1950
8			1575	−288	−1566	1592
9			402	−436	−153	462
10			1291	−433	−1215	1290
11			318	47	−300	304
12			628	35	646	647
13			495	−181	−439	475
14			343	−104	304	322
15			<126	−185	−0	185
16			217	−76	238	250
0	6	1	168	7	0	7
1			3107	−1724	−2388	2945
2			2563	−2448	789	2572
3			1919	−155	1957	1963
4			687	215	583	622
5			1542	−1188	972	1535
6			670	−608	153	627
7			754	−735	−38	736
8			821	−195	803	826
9			1165	1084	396	1154
10			552	532	113	544
11			872	834	155	849
12			<126	58	−17	61
13			209	167	−104	197
14			<109	7	105	105
15			<109	−99	5	99
0	7	1	2220	0	2236	2236
1			2957	2745	−1086	2952
2			2949	−2584	1107	2811
3			1868	−825	1562	1766
4			737	492	−491	695
5			385	−270	286	393
6			946	−42	−931	932
7			1089	−694	−849	1097
8			1114	−230	−1070	1095
9			469	280	−393	483
10			461	−456	−81	463
11			419	−348	−132	372
12			160	39	146	152
13			<118	−63	−73	96
14			285	378	37	380
15			192	−23	−255	256
0	8	1	436	−385	0	385
1			1249	317	−1193	1234
2			1348	−105	1322	1326
3			887	−70	865	868
4			2086	−504	1957	2021
5			301	−164	83	184
6			1274	−768	959	1229
7			209	−233	105	255
8			636	−52	602	604
9			620	−152	561	581
10			921	95	−886	891
11			192	179	45	184
12			268	−17	−224	281
13			126	7	−1	7
14			259	98	−86	131
0	9	1	645	0	−602	602
1			1047	1073	−148	1083
2			939	−2	−881	881
3			1030	173	−1016	1031
4			645	−145	614	631
5			762	−534	582	790
6			695	1	651	651
7			636	−553	−127	568
8			872	−818	25	818
9			620	−54	−598	600
10			251	247	168	298
11			209	162	−17	163
12			185	102	−152	183
13			<109	163	−96	189
14			175	143	−137	198
0	10	1	<134	33	0	33
1			695	716	20	716
2			1089	368	1031	1094
3			1249	548	−1149	1273
4			1005	−953	108	959
5			729	429	530	681
6			377	−379	−4	379
7			335	−175	347	389
8			461	207	−481	523
9			511	−316	398	508
10			310	−352	109	368
11			377	−274	−98	291
12			<118	−222	124	254
13			202	−167	−79	185
0	11	1	478	0	−492	492
1			905	−714	−375	806
2			537	141	−542	560
3			796	−284	−691	747
4			168	−78	209	223
5			168	112	−23	114
6			478	133	482	500
7			562	535	−144	554
8			436	−78	467	474
9			293	116	−287	309
11			217	220	79	234
12			168	78	−145	165
0	12	1	310	−268	0	268
1			234	−224	−72	236
2			620	−306	−518	602
3			343	−53	−347	351
4			552	−34	−525	526
5			<118	69	−10	69
6			453	221	−376	436
7			552	−275	534	601
8			293	−223	−152	269
9			411	−63	−371	376
10			436	−418	163	449
0	13	1	185	0	41	41
1			268	−285	−117	308
2			318	12	229	230
3			562	−424	−323	533
4			268	273	−141	307
5			503	134	−504	522
6			285	−227	−134	263
7			335	202	−243	316
8			352	321	−91	333
9			234	189	171	255
0	14	1	<101	−80	0	80
1			394	−376	207	429
2			285	−318	−25	319
3			369	−333	−145	363
4			185	55	−239	246
5			369	−230	−313	388
6			<101	115	−128	173
7			<84	58	33	67
0	15	1	150	0	196	196
1			<101	229	−234	327
2			<101	82	2	82
3			192	−2	−185	185
4			234	−46	−267	271
0	0	2*	863	965	0	965
1			1700	−1695	0	1695
2			2622	2407	0	2407
3			1600	−1568	0	1568
4			520	271	0	271
5			1767	1762	0	1762
6			1784	−1768	0	1768
7			2346	2301	0	2301
8			1466	−1494	0	1494
9			720	684	0	684
10			<134	−70	0	70
11			628	−636	0	636
12			<143	−59	0	59
13			343	304	0	304
14			<126	−197	0	197
15			<118	147	0	147
16			<109	35	0	35
0	1	2	1893	0	1921	1921
1			4004	1177	3876	4051
2			863	763	470	896
3			2966	395	3173	3197
4			327	−268	−270	380
5			1207	−1051	284	1089
6			3636	2878	−2068	3544
7			1416	−298	1383	1415
8			1315	−604	−1089	1245
9			<134	147	41	152
10			946	−910	−122	919
11			1249	804	−889	1198
12			436	−376	153	406
13			503	−403	−420	583
14			<118	14	34	37
15			301	−46	−349	352
16			202	87	143	168
0	2	2	1081	−1083	0	1083
1			3930	1162	−3874	4045
2			3075	−2149	−2007	2940
3			594	350	−410	539
4			1885	673	1822	1943
5			3602	975	3504	3637
6			2589	469	2488	2532
7			813	848	220	876
8			444	−411	122	429
9			1106	603	972	1144
10			<134	−91	54	106
11			276	113	308	328
12			929	−67	−979	981
13			528	−449	−386	592
14			352	−277	117	301
15			318	120	−321	343
16			168	−28	138	141
0	3	2	2161	0	2085	2085
1			988	136	−899	909
2			1257	−176	−1287	1299
3			2111	98	−2160	2162
4			1709	−69	−1753	1755
5			1944	204	−1976	1986
6			737	740	−3	740
7			369	267	−302	403
8			586	−501	337	604
9			495	364	373	522
10			921	−947	85	950
11			520	328	399	516
12			603	221	−505	551
13			318	−349	−36	350
14			<126	−49	94	106
15			251	173	−166	240
16			150	−75	103	127
0	4	2	3024	−3064	0	3064
1			1508	−1413	29	1413
2			3494	−3373	806	3467
3			2119	1599	1435	2148
4			2463	−1928	1331	2342
5			2170	950	−2012	2225
6			2580	2073	1292	2442
7			301	−340	−183	386
8			1148	1146	47	1147
9			611	−184	552	582
10			<143	186	−82	203
11			394	186	335	383
12			<134	−92	135	163
13			327	−44	−340	343
14			528	−453	−55	456
15			268	10	−187	187
16			<92	51	−34	61
0	5	2	1399	0	−1413	1413
1			3326	−3084	−1331	3359
2			2723	−2718	609	2785
3			3669	1519	−3301	3634
4			2454	−2091	−1304	2465
5			2338	2129	−994	2350
6			1617	−1394	720	1569
7			872	581	−607	840
8			419	449	138	470
9			243	−148	−123	192
10			678	638	−186	665
11			175	−119	140	183
12			670	556	375	670
13			436	418	39	420
14			360	165	−333	372
15			202	−178	−4	178
0	6	2	394	420	0	420
1			2136	−1312	1581	2055
2			1609	−785	1284	1505
3			1047	74	1058	1061
4			1374	−1174	−818	1409
5			2136	−149	−2168	2173

TABLE 8. (*Continued.*)

h	k	l	100kF_o	100A_c	100B_c	100F_c
6	6	2	318	−295	177	345
7			1793	−544	−1733	1816
8			939	−104	933	939
9			209	−48	−132	140
10			<134	−158	93	184
11			175	234	−150	278
12			<126	16	137	138
13			503	300	375	480
14			377	283	−277	396
15			150	−79	150	170
0	7	2	202	0	199	199
1			327	220	−131	256
2			1550	−1301	−746	1500
3			1542	−652	1336	1487
4			1994	−1963	129	1967
5			813	802	129	813
6			385	24	438	439
7			762	422	−664	786
8			946	957	−71	960
9			1013	196	−1009	1028
10			653	705	−163	724
11			453	−47	−403	406
12			343	235	184	299
13			259	172	139	222
14			202	182	12	182
0	8	2	1734	1731	0	1731
1			528	429	−281	513
2			1281	866	−996	1320
3			1977	−1795	−729	1937
4			301	−262	186	322
5			746	−321	−681	752
6			1609	−1574	361	1615
7			276	−50	−335	339
8			1291	−869	1007	1330
9			<134	30	13	32
10			695	−432	−534	687
11			243	244	49	249
12			310	209	−197	287
13			185	28	119	122
14			586	550	269	612
0	9	2	603	0	−564	564
1			1097	1024	473	1128
2			1651	1482	−736	1655
3			1156	−873	695	1116
4			1215	529	1008	1134
5			897	434	816	924
6			754	772	−54	774
7			327	157	−301	340
8			662	669	−182	694
9			887	−326	−835	897
10			293	−154	268	309
11			143	37	−204	207
12			<126	47	11	48
13			126	27	−26	38
0	10	2	209	227	0	227
1			1390	501	−1231	1329
2			887	762	527	927
3			1064	138	−1050	1059
4			444	−418	−123	436
5			402	−347	186	394
6			511	−525	17	525
7			636	−167	542	567
8			259	−152	−249	291
9			185	−84	145	167
10			243	12	223	223
11			160	89	−108	140
12			<109	145	−32	149
0	11	2	704	0	−695	695
1			327	91	−292	306
2			1148	1190	138	1198
3			771	642	−338	726
4			855	864	−131	874
5			168	−230	52	236
6			503	513	−59	517
7			310	217	−140	259
8			436	125	434	452
9			611	−542	184	572
10			259	−78	264	275
11			226	201	115	231
0	12	2	369	−384	0	384
1			419	276	−439	518
2			327	−201	−63	211
3			712	705	−190	730
4			662	504	−505	714
5			402	−416	−90	426
6			293	192	183	265
7			168	−148	169	224
8			160	110	−192	222
9			134	90	−117	148
10			310	232	180	294
0	13	2	636	0	−627	627
1			301	207	−237	315
2			209	13	248	248
3			143	158	22	159
4			259	287	122	312
5			185	−88	−187	207
6			243	−150	128	197
7			<109	−85	103	134
8			118	−6	42	42
0	14	2	226	−294	0	294
1			251	−189	110	219
2			377	167	−296	340
3			150	−13	146	146
4			436	407	127	426
5			150	−10	−138	138
6			276	78	−283	294
0	15	2	202	0	228	228
1			243	55	228	235
2			<92	−140	86	164
1	0	3	1600	0	−1524	1524
2			3971	0	4114	4114
3			1030	0	1034	1034
4			4189	0	4272	4272
5			552	0	513	513
6			335	0	−189	189
7			310	0	−321	321
8			486	0	−463	463
9			887	0	−852	852
10			234	0	−235	235
11			419	0	−462	462
12			729	0	−743	743
13			<126	0	33	33
14			<109	0	−12	12
15			<126	0	78	78
16			<92	0	55	55
0	1	3	6936	0	−7029	7029
1			594	527	−278	596
2			846	131	−855	865
3			411	76	354	362
4			754	−51	780	782
5			1039	104	1090	1095
6			1064	71	1090	1092
7			872	−529	−588	791
8			963	−500	804	947
9			259	−174	−174	246
10			293	10	292	293
11			662	541	−268	604
12			469	417	237	480
13			385	328	142	358
14			301	222	−187	290
15			217	93	61	111
16			<92	−73	−78	107
0	2	3	1944	1926	0	1926
1			2412	−1340	−2009	2415
2			1215	158	1171	1182
3			1717	1593	552	1686
4			1365	−1197	537	1312
5			1986	1661	850	1866
6			921	650	667	931
7			1030	716	−700	1002
8			486	−450	−5	450
9			402	−310	12	310
10			268	−113	235	261
11			872	−865	−160	880
12			202	−30	−269	270
13			160	−67	−103	123
14			217	181	23	182
15			259	212	−79	226
16			175	168	129	212
0	3	3	4516	0	−4472	4472
1			1416	−1438	−119	1443
2			3142	2421	−1935	3099
3			444	408	106	421
4			1249	1148	418	1222
5			537	−466	237	523
6			1173	366	1106	1165
7			1784	1663	−579	1761
8			1315	−742	1120	1343
9			1441	1432	39	1432
10			796	−251	763	803
11			268	8	159	160
12			343	329	42	332
13			285	−229	−60	236
14			234	202	−118	234
15			285	−213	−91	232
0	4	3	268	−260	0	260
1			1767	705	−1558	1710
2			3107	25	−3115	3115
3			486	−435	−253	504
4			1416	−626	−1417	1549
5			653	−529	−305	611
6			636	285	143	319
7			729	−367	596	700
8			1064	893	698	1133
9	4	3	318	171	315	359
10			419	−133	345	369
11			335	326	−203	384
12			754	−16	765	765
13			343	72	−340	347
14			126	−64	95	115
15			185	88	152	176
0	5	3	2622	0	2535	2535
1			720	−207	−639	671
2			1207	1197	−102	1201
3			1567	326	−1445	1481
4			921	507	−742	899
5			1131	1039	−334	1091
6			520	−506	−287	582
7			620	515	346	621
8			1106	1081	−105	1086
9			887	941	−54	942
10			511	−124	516	531
11			804	−558	613	829
12			310	−47	263	268
13			259	−213	80	227
14			<126	8	−104	104
15			160	−102	−136	170
0	6	3	914	−897	0	897
1			1148	−1050	−470	1151
2			522	−152	−495	518
3			2018	−1973	98	1975
4			653	150	583	602
5			1809	−1619	−660	1748
6			444	386	−110	401
7			729	−743	143	757
8			1333	1313	150	1322
9			569	323	−510	603
10			552	−41	532	533
11			611	648	−101	656
12			670	−501	438	666
13			352	264	229	349
14			134	−16	−16	22
0	7	3	2178	0	2194	2194
1			1474	1378	−561	1488
2			887	−604	666	899
3			1441	1298	428	1367
4			939	−941	−187	960
5			310	213	−207	297
6			234	156	10	157
7			804	−750	−300	808
8			1022	931	−442	1031
9			1165	−1087	404	1160
10			301	298	−86	310
11			436	34	483	484
12			343	−119	263	289
13			150	−18	172	173
14			134	187	45	192
0	8	3	<134	184	0	184
1			1357	−581	1265	1392
2			1013	128	1003	1011
3			1240	−937	−827	1250
4			1306	1089	801	1352
5			746	27	−742	743
6			537	−270	470	542
7			762	−388	−714	813
8			394	−135	−362	387
9			202	−113	182	214
10			495	417	187	457
11			<109	3	43	43
12			318	−206	−176	271
13			444	−352	258	437
0	9	3	<134	0	216	216
1			1491	1512	−21	1512
2			<126	−56	−63	84
3			946	163	856	871
4			804	−668	539	858
5			537	−393	432	584
6			687	143	656	671
7			579	−468	−174	500
8			276	14	249	250
9			737	−671	410	787
10			586	616	−104	624
11			<134	−32	18	37
12			<118	6	−43	44
0	10	3	520	542	0	542
1			603	−199	585	618
2			1005	995	−68	996
3			956	795	−569	978
4			444	−169	−392	426
5			620	564	−185	593
6			503	−439	−107	452
7			268	−264	−135	296
8			185	−26	170	172
9			419	−411	206	459
10			461	368	−326	492
11			520	−494	76	500

TABLE 8. (*Continued.*)

h	k	l	100kF_o	100A_c	100B_c	100F_c
0	11	3	259	0	−268	268
1			678	−199	660	689
2			897	−813	470	939
3			411	−344	59	349
4			276	192	133	234
5			461	−45	456	458
6			552	337	488	593
7			202	132	18	134
8			276	−22	205	206
9			<126	111	−44	119
10			<109	−71	−97	121
0	12	3	268	−308	0	308
1			301	184	−187	262
2			528	437	−161	466
3			453	484	262	551
4			939	143	−925	936
5			<118	−167	39	171
6			259	7	−313	313
7			<126	−52	178	186
8			<109	7	121	122
9			150	−143	−154	210
0	13	3	695	0	673	673
1			603	−596	176	621
2			495	−421	243	486
4			369	326	163	364
5			251	157	−201	255
6			160	−170	−94	194
7			175	171	−4	171
0	14	3	352	371	0	371
1			310	293	181	344
2			160	−209	−97	231
3			226	−272	89	286
4			134	154	−23	155
0	0	4	687	657	0	657
1			1658	−1600	0	1600
2			2814	2780	0	2780
3			1340	−1304	0	1304
4			670	703	0	703
5			461	−431	0	431
6			444	−419	0	419
7			1340	−1392	0	1392
8			1223	−1278	0	1278
9			552	534	0	534
10			444	−564	0	564
11			478	477	0	477
12			562	546	0	546
13			168	−55	0	55
14			234	227	0	227
15			<92	1	0	0
0	1	4	1432	0	1427	1427
1			1776	880	1375	1632
2			1215	1164	333	1211
3			1986	163	2015	2022
4			1734	1513	−821	1721
5			2496	360	2524	2550
6			327	−333	−215	397
7			1223	−1203	224	1224
8			788	−97	744	750
9			771	−267	−728	775
10			628	−512	388	642
11			226	−174	−27	176
12			268	−190	255	319
13			293	282	−66	290
14			143	−134	−60	147
15			150	59	23	64
0	2	4	1641	1606	0	1606
1			2102	−1170	−1926	2254
2			1264	435	1217	1292
3			788	−658	−411	776
4			603	−394	466	610
5			1114	−60	1134	1135
6			453	118	−373	391
7			2405	−213	2454	2463
8			327	223	204	302
9			202	−183	−19	184
10			444	189	−428	468
11			251	−57	−205	213
12			<118	−21	102	104
13			192	−133	−195	235
14			<118	66	34	75
15			126	−64	−135	150
0	3	4	653	0	−662	662
1			1860	1064	−1492	1833
2			1022	792	−693	1006
3			1232	381	−1212	1271
4			1609	1411	685	1568
5			528	−409	−382	560
6			1668	−334	1537	1573
7			779	−297	777	832
8			611	−518	−22	518
9			921	−863	228	892
10			880	−879	276	922
11			301	−193	−167	255
12			185	−171	79	188
13			352	145	303	336
14			234	38	−205	209
15			126	48	63	79
0	4	4	855	−794	0	794
1			695	428	−512	668
2			1843	−1740	−456	1799
3			377	−308	−31	310
4			1424	458	−1323	1400
5			1291	551	1109	1238
6			929	824	340	891
7			1123	481	972	1084
8			838	803	−362	881
9			971	−938	−196	958
10			444	457	97	467
11			670	−509	−396	645
12			175	−27	92	96
13			175	−234	8	234
14			192	−105	168	198
0	5	4	771	0	751	751
1			<118	−132	−72	150
2			678	653	−160	672
3			804	−570	−692	896
4			1340	−1171	669	1349
5			1885	272	−1891	1910
6			1123	−971	598	1140
7			579	551	61	554
8			662	−680	−54	683
9			863	−606	549	818
10			251	267	83	279
11			318	−130	188	228
12			168	183	−77	199
13			143	−75	106	130
14			109	101	−131	166
0	6	4	887	−893	0	893
1			1097	89	1136	1139
2			1634	−432	−1589	1647
3			495	533	48	535
4			1081	493	−964	1083
5			327	−412	−8	412
6			720	480	−512	702
7			804	−672	−480	825
8			369	−59	345	350
9			<134	80	149	169
10			268	−172	−13	173
11			385	−158	−395	426
12			<109	104	81	132
13			126	−108	47	118
0	7	4	1173	0	1104	1104
1			746	−380	662	763
2			1550	83	1600	1602
3			887	−860	38	861
4			1005	−924	−416	1013
5			461	455	−128	472
6			729	−383	−570	687
7			310	−265	−107	286
8			226	−180	94	203
9			<118	14	69	71
10			461	265	−396	476
11			185	−78	−141	161
12			<118	187	−35	190
13			143	−82	−118	144
0	8	4	411	385	0	385
1			813	−359	−725	809
2			855	835	−53	837
3			796	1	818	818
4			394	−167	−369	405
5			427	−399	98	411
6			478	−373	−133	396
7			343	−161	−330	367
8			586	−518	78	524
9			495	392	163	425
10			453	−64	−416	421
11			143	−61	123	137
12			192	38	−206	209
0	9	4	569	0	514	514
1			545	−440	296	531
2			202	25	193	195
3			<134	36	127	133
4			687	523	412	665
5			411	−295	200	356
6			503	419	−248	487
7			444	−381	−177	420
8			453	239	−407	472
9			310	−303	111	323
10			377	−310	−197	367
11			<101	93	−6	93
0	10	4	<118	−23	0	23
1			1047	640	−823	1042
2			929	251	850	887
3			251	−159	218	270
4	10	4	<126	91	19	93
5			318	283	54	289
6			226	−242	−45	246
7			461	303	326	445
8			335	6	−314	314
9			276	−178	199	267
10			377	57	−315	320
0	11	4	243	0	−204	204
1			603	−360	−498	615
2			411	282	−331	434
3			360	−207	−257	330
4			452	459	92	469
5			268	−266	−34	268
6			217	215	71	226
7			175	−107	−121	162
8			126	61	−71	94
9			126	−58	27	64
0	12	4	<101	−78	0	78
1			285	147	207	254
2			276	−216	−31	218
3			579	557	−20	557
4			209	68	−65	94
5			143	59	−75	96
6			126	144	59	155
7			150	94	−47	105
0	13	4	670	0	−730	730
1			360	−185	−327	376
2			310	−306	34	308
3			318	−353	−98	366
4			160	−140	−72	157
5			92	−107	−26	110
1	0	5	1390	0	1396	1396
2			796	0	832	832
3			762	0	781	781
4			318	0	−277	277
5		*	1725	0	−1720	1720
6			1232	0	1228	1228
7			<134	0	−146	146
8			1190	0	−1150	1150
9			202	0	153	153
10		*	838	0	−751	751
11			251	0	310	310
12			444	0	−460	460
0	1	5	1348	0	−1272	1272
1			1165	1018	449	1113
2			846	−195	−808	831
3			1291	−281	1282	1313
4			1793	−1778	62	1779
5			2052	−1947	39	1948
6			1508	−1342	646	1489
7			762	−300	−660	725
8			788	777	179	797
9			562	−545	−215	586
10			192	233	17	234
11			<118	−75	−55	93
12			134	142	67	157
13			192	157	−66	171
0	2	5	495	496	0	496
1			628	628	37	629
2			720	623	304	693
3			1626	1589	84	1592
4			712	705	148	721
5			813	795	48	796
6			1843	−1360	−1138	1773
7			929	994	−78	997
8			1181	−1033	−465	1133
9			343	−4	389	389
10			243	146	−165	220
11			594	−623	8	623
12			185	178	0	178
13			185	−62	102	119
14			217	231	−115	258
0	3	5	956	0	−967	967
1			939	−940	−96	945
2			586	285	−546	616
3			1458	−963	1046	1422
4			1165	−353	−1126	1180
5			897	896	−8	896
6			779	616	77	779
7			929	−443	−935	1034
8			552	−133	547	563
9			453	215	−323	388
10			185	−128	154	201
11			<109	−40	−57	69
12			209	−194	−115	226
13			<101	48	22	53
0	4	5	160	162	0	162
1			1257	392	−1177	1241
2			1139	419	−1076	1155
3			887	921	29	922
4			385	−160	−334	371
5			887	235	833	865

TABLE 8. (*Continued.*)

h	*k*	*l*	100kF_o	100A_c	100B_c	100F_c
6	4	5	1508	−1015	−1109	1503
7			436	409	220	465
8			226	−142	116	183
9			385	248	318	404
10			419	309	247	396
11			<109	−15	−73	74
12			175	−46	105	115
13			<92	−27	33	42
0	5	5*	863	0	841	841
1			804	−781	−240	817
2			<126	36	−14	39
3			1190	−395	−1090	1160
4			971	944	−217	968
5		*	537	17	−344	345
6			1039	537	−850	1005
7			478	406	−237	471
8			528	−338	−379	508
9			444	444	−5	444
10		*	243	−205	−1	205
11			150	−6	170	170
12			160	54	−95	110
13			301	−282	−43	285
0	6	5	687	−644	0	644
1			310	−324	−33	326
2			369	364	−43	367
3			1449	−1406	135	1413
4			419	−284	266	389
5			436	335	158	371
6			444	−153	345	377
7			318	254	46	258
8			419	327	165	366
9			444	369	−184	412
10			185	6	80	81
11			285	199	−6	199
12			160	−69	−107	127
0	7	5	788	0	772	772
1			<126	−119	−31	122
2			<126	−86	15	87
3			720	649	−251	696
4			327	321	−97	335
5			327	−234	−146	276
6	7	5	695	5	−671	671
7			259	−195	−171	259
8			377	−80	−372	380
9			209	−119	131	177
10			175	76	−197	211
11			209	−87	183	203
0	8	5	436	444	0	444
1			620	−418	483	638
2			729	27	785	785
3			<126	−75	77	107
4			469	129	460	478
5			243	−99	−239	259
6			520	90	526	534
7			318	55	−271	276
8			160	−177	24	178
9			419	312	−230	387
10			285	−230	−200	305
11			<84	82	35	89
0	9	5	251	0	−282	282
1			217	228	−103	250
2			<118	35	−96	103
3			653	152	672	689
4			653	226	−598	639
5			419	−142	393	417
6			134	135	138	193
7			<101	−77	−23	81
8			<118	−38	81	90
9			192	−213	18	214
10			92	−76	94	121
0	10	5	511	524	0	524
1			<109	−15	−110	111
2			<109	127	−28	130
3			343	353	108	369
4			134	−78	70	104
5		*	335	201	255	324
6			209	−94	193	215
7			<118	129	17	130
8			<92	−28	0	28
9			217	−186	−70	199
0	11	5	469	0	−477	477
1			234	−170	−32	173
2	11	5	495	294	−404	500
3			318	−268	40	271
4			243	245	80	257
5			427	300	301	425
6			168	150	131	199
7			226	66	172	184
0	12	5	327	−330	0	330
1			<109	44	−77	89
2			327	−93	−317	331
3			<92	−49	−68	84
4			217	−43	−206	210
5			251	58	270	276
0	0	6	897	848	0	848
1			695	−730	0	730
2			921	965	0	965
4			461	515	0	515
5			552	−521	0	521
8			712	−747	0	747
9			628	605	0	605
10			444	−497	0	497
11			569	575	0	575
0	1	6	569	0	562	562
	3		712	0	−709	709
	4		997	−976	0	976
	5		704	0	−703	703
	8		552	604	0	604
1	0	7	636	0	626	626
3			897	0	928	928
6			192	0	258	258
7			662	0	−645	645
0	1	7	411	0	−455	455
	2		486	444	0	444
	4		813	−883	0	883
	5		419	0	435	435
	6		1097	−1114	0	1114
	7		301	0	338	338
0	0	8	168	212	0	212
1			276	−273	0	273
2			234	241	0	241

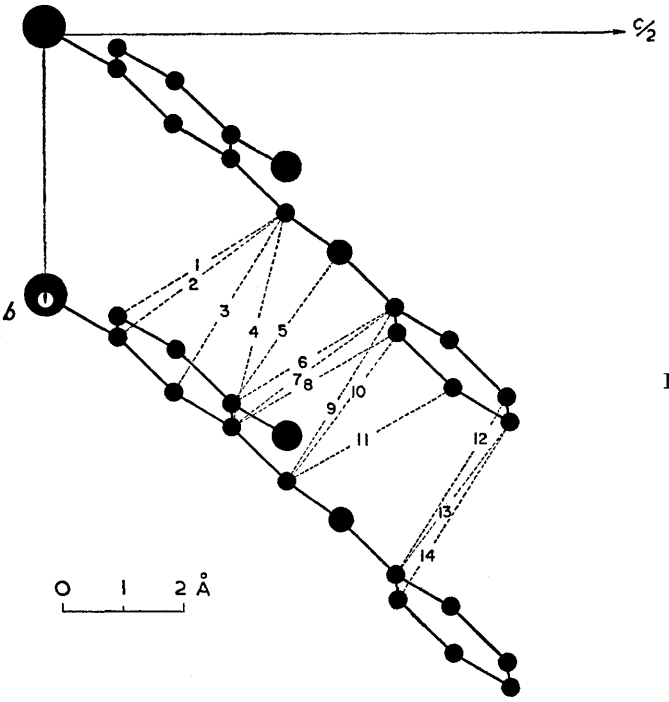


FIG. 4c. *N*-5-Chlorosalicylideneaniline; packing diagram seen along [100], showing two molecules only. For contact distances see Table 11.

low remperature, to within 1° of their respective normals. The nitrogen is displaced by 0·1 Å from the plane of ring A, which corresponds to a stepping of the aldehyde and anil rings across the C=N bond. This deviation from molecular planarity may be viewed as partly relieving repulsion between H_9 and H_7; the in-plane deformation around C_8 ($\widehat{NC_8C_9} = 124°$) and the rotation of approximately 5° about bonds C_1–C_7 and N–C_8 operate in the same direction to produce a H_9–H_7 separation of 2·0 Å.

The packing arrangement of the 5′-chloroanil is characteristic of flat molecules arranged in stacks along the shortest axis, in which the molecules are inclined at about 40° to (010); within

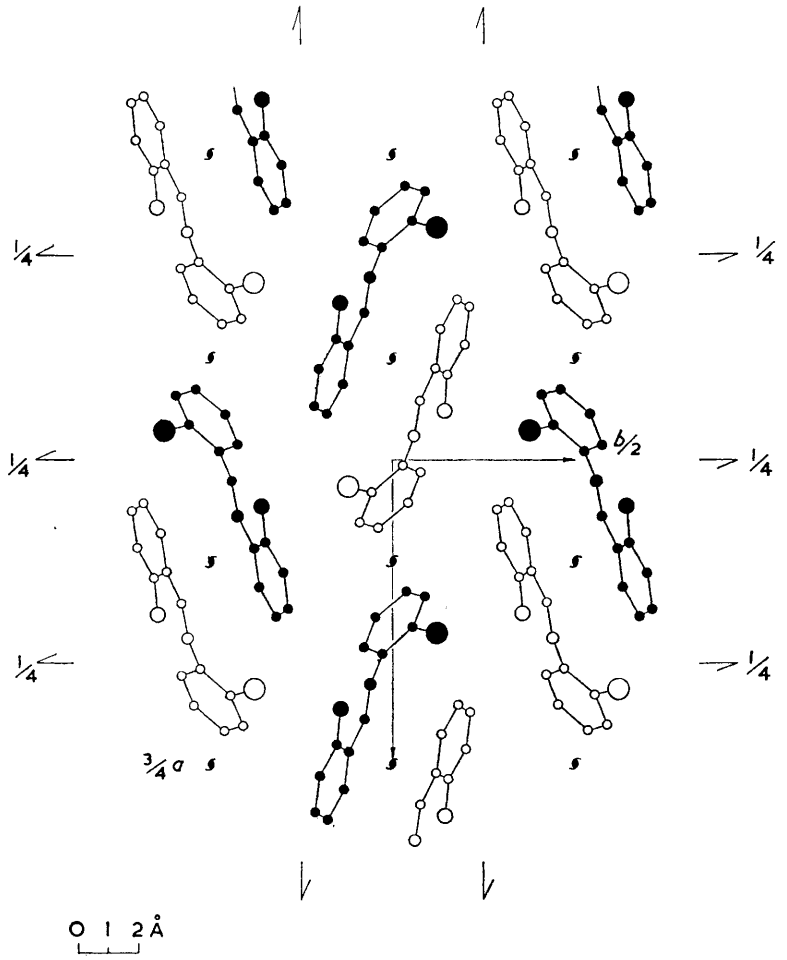


FIG. 5a. 2-Chloro-*N*-salicylideneaniline; packing diagram seen along [001].

each stack they are held at an interplanar distance of 3·4 Å. Packing diagrams are given in Fig. 4 where intermolecular van der Waals contacts of less than 3·7 Å are shown. Rotation of the anil ring in the 2-chloro-derivative prevents any such close parallel stacking. Packing diagrams of the latter seen along [001] and [010] are shown in Fig. 5. The plane C_1–C_7,N lies roughly parallel to (101) with molecules making close contact across twofold screw axes parallel to [001] (Table 9a). Close contacts between nearest-neighbour molecules related by translation in the *c*-direction, and twofold screw axes along [100] and [010] are given in Tables 9b—d, respectively.

Table 10 lists the bond lengths of the two anils. In neither structure does the variation in bond

TABLE 9.

Intermolecular distances (Å).

(*a*)	(*b*)	(*c*)	(*d*)
$C_2 \cdots C_3$ 3·57	O $\cdots$ C_5 3·31	$C_5 \cdots H_{11}$ 3·02	$C_8 \cdots H_2$ 2·81
$C_2 \cdots H_3$ 3·05	Cl $\cdots$ C_4 3·60	$C_6 \cdots H_{11}$ 2·99	$C_9 \cdots H_2$ 3·04
N $\cdots$ H_{11} 2·87	O $\cdots$ H_5 2·62		$C_{12} \cdots H_3$ 2·96
Cl $\cdots$ H_{10} 3·02			$C_{13} \cdots H_2$ 2·94
Cl $\cdots$ H_{11} 3·11			
$C_1 \cdots C_{11}$ 3·56			
$C_1 \cdots H_{11}$ 3·06			
$C_6 \cdots C_{11}$ 3·56			
$C_7 \cdots C_{12}$ 3·54			

lengths in the benzene rings conform to a clear or interpretable pattern, nor can we account for the variation of bonds C_5–C_6, C_{11}–C_{12}, and C_{12}–C_{13} with temperature in the 5′-chloroanil. The mean C–H bond length of the 2-chloroanil is 1·04 ± 0·05 Å. The mean e.s.d. of these bond

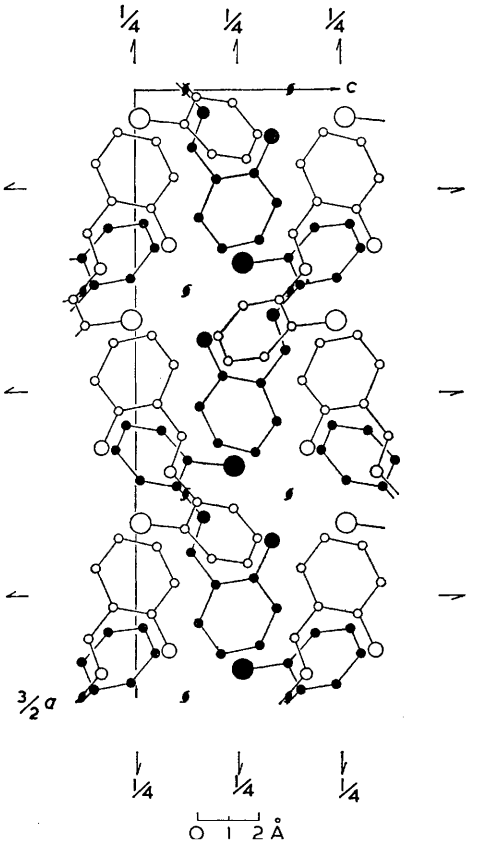


FIG. 5b. 2-Chloro-*N*-salicylideneaniline; packing diagram seen along [010].

lengths is 0·03 Å. Corresponding values for the 5′-chloroanil are 0·99 ± 0·05 Å, and 1·02 ± 0·04 Å at room and low temperature. We note the equality of the exocyclic C_8–N bond in the three structures. The mean value of 1·418 Å compares with the length (1·426 Å) of the corresponding bond in acetanilide.[7] The exocyclic C_1–C_7 bonds in the 5′-chloroanil are equal (mean value of 1·441 Å) and do not differ appreciably from the corresponding bond in the 2-chloroanil (1·452 Å). These lengths can be compared to values of 1·506 Å in *o*-nitrobenzaldehyde,[8] 1·48 ±

[7] Brown and Corbridge, *Acta Cryst.*, 1954, **7**, 711.
[8] Coppens and Schmidt, *Acta Cryst.*, 1964, **17**, in the press.

0·016 Å in benzoic acid,[9] 1·474 Å in 5-chlorosalicylaldoxime,[10] 1·458 Å in salicyclic acid,[11] 1·44 Å in copper salicylate tetrahydrate,[12] and 1·44 ± 0·014 Å and 1·40 ± 0·013 Å in 2- and 1-naphthoic acids,[13] respectively. The wide spread of this bond length makes discussion difficult. The scatter in length of the three C–O bonds is almost within their standard deviations. The mean value (1·362 Å) compares well with the C–O bond length in salicyclic acid (1·361 Å). The difference in length between the mean value of the 5′-chloroanil C–Cl bond (1·756 Å) and the corresponding 2-chloroanil bond (1·737 Å) is probably significant; we compare these results with similar lengths in 5-chlorosalicylaldoxime, 1·777 Å, and in *o*-chlorobenzoic acid,[14] 1·737 Å.

We next draw attention to the problem of the pure C=N bond. Cox and Jeffrey in 1951 [15] reported: " There is no direct experimental evidence on the C=N double-bond length and there are indeed few molecules on which it might be measured; *O*-ethers of oximes, $R_1R_2C{:}NOR$ should possess unequivocal double bonds but none has yet been studied. A recent *X*-ray investigation of acetoxime . . . gives N=C = 1·31 Å but the occurrence of a well-marked system of N · · · H · · · O bonds between adjacent molecules in this structure suggests caution in accepting either N=C or N–O as bonds of integral order; 1·31 Å is somewhat higher than would be expected for a pure N=C double bond. The covalent radii values of Stevenson and Schomaker with the electronegativity correction according to Gordy give 1·27 Å which is also the mean of the O=O and C=C lengths. Interpolation between C–N and C=N [C≡N? B., L., O.] lengths, assuming analogy with carbon–carbon bonds, indicates 1·28—1·29 Å. We therefore take 1·28 Å as the N=C double-bond length in this discussion." A recent structure

TABLE 10.

Comparison of bond lengths (Å).

	Ring A (aldehyde moiety)				Ring B (aniline moiety)				
	Room temp.*	Room temp.†	Low temp.‡	2-Chloro-anil *		Room temp.*	Room temp.†	Low temp.‡	2-Chloro-anil *
C_1–C_2 ...	1·418	1·423	1·416	1·391	C_8–C_9 ...	1·410	1·415	1·415	1·384
C_2–C_3 ...	1·398	1·399	1·392	1·394	C_9–C_{10} ...	1·367	1·368	1·370	1·369
C_3–C_4 ...	1·363	1·366	1·379	1·388	C_{10}–C_{11}	1·386	1·390	1·401	1·379
C_4–C_5 ...	1·405	1·411	1·400	1·368	C_{11}–C_{12}	1·372	1·377	1·409	1·376
C_5–C_6 ...	1·360	1·361	1·385	1·385	C_{12}–C_{13}	1·404	1·405	1·385	1·391
C_6–C_1 ...	1·407	1·411	1·412	1·400	C_{13}–C_8 ...	1·387	1·391	1·400	1·381
r.m.s. ...	1·392	1·395	1·397	1·388	r.m.s. ...	1·388	1·392	1·397	1·380
					C_1–C_7 ...	1·444	1·445	1·438	1·452
					C–O	1·351	1·356	1·364	1·365
					C=N ...	1·270	1·273	1·292	1·288
					N–C ...	1·419	1·420	1·414	1·421
					C–Cl ...	1·755	1·759	1·752	1·737
					O · · · N	2·584		2·594	2·609

* Bond lengths uncorrected for thermal vibrations. † Bond lengths corrected for thermal vibrations. ‡ Maximum bond-length correction for thermal vibrations = 0·001 Å.

TABLE 11.

Short intermolecular contact distances (Å) (see Fig. 4). (Low-temperature structure.)

1′	3·50	1	3·62	6	3·54	11	3·48
2′	3·67	2	3·48	7	3·35	12	3·55
3′	3·40	3	3·51	8	3·54	13	3·30
4′	3·47	4	3·70	9	3·42	14	3·57
5′	3·62	5	3·30	10	3·26		

analysis of 2-methylthiobenzothiazole [16] reports a C=N bond length of 1·27 Å; however, the estimated limits of accuracy of 0·05 Å are too high for our present purpose; 5-chlorosalicyl-aldoxime [10] has been found to contain a C=N bond of length 1·237 Å which the authors consider

[9] Sim, Robertson, and Goodwin, *Acta Cryst.*, 1955, **8**, 157.
[10] Simonsen, Pfluger, and Thompson, *Acta Cryst.*, 1961, **14**, 269.
[11] Cochran, *Acta Cryst.*, 1953, **6**, 260.
[12] Hanic and Michalov, *Acta Cryst.*, 1960, **13**, 299.
[13] Trotter, *Acta Cryst.*, 1961, **14**, 101; 1960, **13**, 732.
[14] Ferguson and Sim, *Acta Cryst.*, 1961, **14**, 1262.
[15] Cox and Jeffrey, *Proc. Roy. Soc.*, 1951, *A*, **207**, 110.
[16] Wheatley, *J.*, 1962, 3636.

to be " a little short." An estimate of $1{\cdot}26_5$ Å for the length of the pure C=N double bond is given by Levine,[17] on the basis of microwave studies on the monomeric formaldoxime.

We assume tentatively that the C=N bond-length values (1·292 and 1·273 Å corresponding to the low- and room-temperature structures of the 5′-chloroanil, whose difference amounts to three times the standard deviation of the measurement, represent a significant variation of this bond length with temperature and indicate a weakening of the O • • • N hydrogen bond with increasing temperature. This assumption is in accord with our results on the variations of electron density with temperature in the O • • • N region of the 5′-chloroanil; it is further supported by the results on the 2-chloroanil in which both the electron-density distribution in the O • • • N region and the C=N bond length agree with the corresponding low-temperature data of the 5′-chloroanil.

The value of 1·273 Å need not yet be accepted as the true length of the C=N bond of order two since the O • • • H • • • N bond though weakened is still present in the room-temperature structure of the 5′-chloroanil. For a determination of the unmodified C=N bond length we suggest as suitable materials the centric Schiff bases, the *p*-toluidine dianil of terephthaldehyde (a = 18·3, b = 7·8, c = 6·1 Å, β = 107·5°, $P2_1/a$, n = 2, $d_{calc.}$ = 1·24 g./cm.^{3}), and *NN*′-di-*p*-methylbenzylidene-*p*-phenylenediamine (a = 19·5, b = 7·0, c = 6·5 Å, β = 108°, $P2_1/a$, n = 2, $d_{calc.}$ = 1·22 g./cm.^{3}).

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[17] Levine, *J. Chem. Phys.*, 1963, **38**, 2328.