391. *Topochemistry. Part IX.* The Crystal and Molecular Structures of* N-5-*Chlorosalicylideneaniline near* 90 *and* 300°K.

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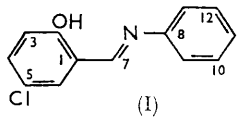
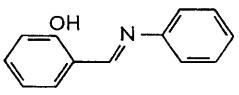
The crystal structure of *N*-5-chlorosalicylideneaniline has been solved by Patterson methods from partial three-dimensional, photographic data collected at 300 and 90°K. The co-ordinates of carbon, nitrogen, oxygen, and chlorine have been located by an anisotropic least-squares refinement with an accuracy of at least 0·006 and 0·007 Å at room and low temperature, respectively. The positional and isotropic temperature parameters of the hydrogen atoms attached to carbon have also been derived. The electron-density distribution in the O · · · N region has been determined by three-dimensional difference syntheses; at low temperature a single peak of 0·5 e/Å^3 corresponds to hydrogen attached to oxygen; the room-temperature distribution shows two peaks (0·25 e/Å^3 each), one of which is identified as the hydroxylic hydrogen.

The thermal vibrations have been analysed in terms of rigid-body motion. Molecular shape, packing arrangement, and bond lengths are discussed in the following Paper (Part X).

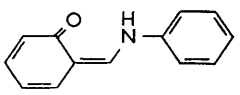
The structure analyses of *N*-5-chlorosalicylideneaniline (I) † at room temperature and near the temperature of boiling nitrogen form part of a research programme on the photochemistry of the anils of salicylaldehyde. It has been shown (Part VI [1]) that the crystalline anils fall into two classes defined by their behaviour on irradiation with ultraviolet light (3600 Å). The first class develops an absorption band with a maximum near 4800 Å which can be eradicated thermally or by irradiation within this new band (reversible photochromy). To this class belongs 2-chloro-*N*-salicylideneaniline whose crystal structure will be described in the following Paper. The second class of solid anils does not colour in light, *i.e.*, is not photochromic; on the other hand, all members of this class show a more or less intense absorption band similar in position to the "photochromic" band mentioned above. In a sub-class characterised by a shortest axis of 4·6 ± 0·1 Å (see



(I)



(II)



(III)

Table 2, Part VI), which includes *N*-5-chlorosalicylideneaniline, this band is sufficiently intense to impart to the crystals a red colour as against the yellow tinge of the majority of solid anils. This absorption band at 4800 Å has been shown to decrease with decreasing temperature and to vanish at the temperature of liquid air. The resultant colour change red ⇌ yellow is reversible in all compounds investigated (reversible thermochromy). Spectroscopic evidence presented in Parts VI and VIII is interpreted in terms of a tautomeric equilibrium (II) ⇌ (III).

It has further been shown that photochromy and thermochromy are mutually exclusive properties: they are determined not by the molecular species as such but by its crystal structure, for several anils occur in dimorphs of which one is thermochromic while the other is photochromic.

X-Ray structure analyses of salicylideneanilines have been carried out for two purposes: first, we compare the detailed features of the molecular structures and packing arrangements in thermochromic and photochromic crystals; secondly, we compare the structures of a thermochromic anil at two temperatures corresponding to bleaching and to maximum

* Part VIII, preceding Paper.

† Numbering shown is that used in the crystallographic descriptions and in bond dimensions.

[1] Part VI, *J.*, 1964, 2041.

coloration (low and high temperatures, respectively). Spectroscopic data indicate that in (I) the thermochromic band at 4800 Å has completely disappeared at 90°K while at room temperature conversion to the coloured form amounts to approximately 50% of the maximum obtainable just below the melting point (110°). The absolute concentration of the coloured species is, however, not known.

Experimental

N-5-Chlorosalicylideneaniline, $C_{13}H_{10}ClON$, *M* 231·7, crystallises from dioxan in red orthorhombic needles elongated along [010] and showing {100} and {001}. The cell dimensions were obtained at the two temperatures from high-order reflections on calibrated Weissenberg zero-level photographs; at room temperature: $a = 12{\cdot}319$, $b = 4{\cdot}527$, $c = 19{\cdot}48$ Å; at low temperature: $a = 12{\cdot}175$, $b = 4{\cdot}480$, $c = 19{\cdot}25$ Å (estimated error 0·1%). The changes in cell dimensions are no more than would be expected from normal thermal coefficients of expansion. *Absences:* $0kl$ for l odd, $h0l$ for h odd. *Space group:* $Pca2_1$ or $Pcam$. $d_{calc.}$, for $n = 4$, 1·417 g./cm.^{3}. $\mu = 30{\cdot}0$ cm.$^{-1}$; $F(000) = 480$. The higher-symmetry space group is ruled out by packing considerations; $Pca2_1$ was adopted, and proved correct by the eventual refinement.

Well-exposed photographs at either temperature show no signs of a superlattice nor any other abnormal features. Photographs of a large crystal taken with Mo-Kα radiation do not indicate any peculiarities in the range beyond the Cu-Kα sphere. Indeed, the similarities of photographs taken at the two temperatures suggest that any differences in structure produced by variations in temperature are minor.

Intensities of the $h0l$, $h1l$, $h2l$, and $h3l$ levels were collected with Cu-Kα radiation on an equi-inclination Weissenberg camera with the multiple-film technique from a cylindrically-shaped crystal of diameter 0·29 mm.; the $0kl$ intensities were taken from a crystal cut to an approximate cylinder elongated along [100]. Low-temperature data were taken by means of the device described by Hirshfeld and Schmidt.[2]

The intensities (hkl and $hk\bar{l}$) were estimated on two sets of six films exposed for approximately 24 and 3 hr., respectively; on the upper-level photographs only the extended spots were read. Reflections, " unobserved " on the strongest films were assigned intensities equal to the lowest value read on this film. Information on the intensity data is listed in Table 1. The averaged film readings were corrected for the Lorentz and polarisation factors, spot extension,[3] and absorption.[4]

Table 1.

Intensity data.

	Low temperature		Room temperature	
	Reflections	Unobserved reflections	Reflections	Unobserved reflections
$h0l$	150	1	156	3
$h1l$	302	5	310	23
$h2l$	273	2	278	20
$h3l$	230	9	238	16
Total	955	17	982	62

Solution of the Structure.—The Patterson projection $P(xz)$ was computed and yielded both the x parameter of the chlorine atom and approximate x,z parameters of the light atoms. The trial model was successfully refined by means of our standard least-squares programme (see Part V [5]). The weighting factors $w(hkl)$ employed in this analysis varied approximately as F_o^{-3}, but were modified in accordance with the number of observations of each reflection and their estimated reliabilities. " Unobserved " reflections were given weight ½ relative to observed reflections of equal magnitude; the programme included these reflections in the refinement cycle only if $|F_c| > kF_{threshold}$. The following scattering-factor curves were used: f_{Cl} Dawson,[6] $f_{C,N,O}$ Berghuis *et al.*,[7] f_H McWeeny.[8] No allowance was made for anomalous-dispersion effects of the chlorine atom.

[2] Hirshfeld and Schmidt, *Acta Cryst.*, 1956, **9**, 233.
[3] Philips, *Acta Cryst.*, 1956, **9**, 819.
[4] Bond, International Tables for *X*-ray Crystallography, Vol. II, ed. Kasper and Lonsdale, Kynoch Press, Birmingham, 1959, p. 295.
[5] Part V, *J.*, 1964, 2030.
[6] Dawson, *Acta Cryst.*, 1960, **13**, 403.
[7] Berghuis, Haanappel, Potters, Loopstra, MacGillavry, and Veenendaal, *Acta Cryst.*, 1955, **8**, 478.
[8] McWeeny, *Acta Cryst.*, 1951, **4**, 513.

During the first few cycles all atoms were treated isotropically; later, all hydrogens attached to carbon were located from a difference synthesis $\delta(xz)$ and inserted into the structure-factor calculations; subsequently, all atoms except hydrogen were assigned anisotropic temperature factors. The low-temperature $F(h0l)$ data were treated by an identical procedure based on the best x,z co-ordinates derived from the room-temperature data.

Next $P(yz)$ was computed to locate the y parameter of chlorine; however, overlap made this projection intractable. Attempts to determine y parameters from packing considerations alone also failed.

A generalised Patterson line synthesis along $(x,\frac{1}{2})$ (Fig. 1) was computed from the scaled $F^2(h1l)$, and interpreted as follows: this function contains the chlorine–chlorine vectors $(2x,2y,\frac{1}{2})$ and $(\frac{1}{2}\text{-}2x,0,\frac{1}{2})$ at $(2x,\frac{1}{2})$ and $(\frac{1}{2}\text{-}2x,\frac{1}{2})$ such that the height of the former peak (M) is modified by $\cos 2\pi 2y$ while the latter peak (U) is unmodified. A comparison of the two peak heights should therefore give y_{Cl}. However, while the two peaks were located on the line synthesis at the expected x co-ordinates they proved to lie in regions of high and low background,

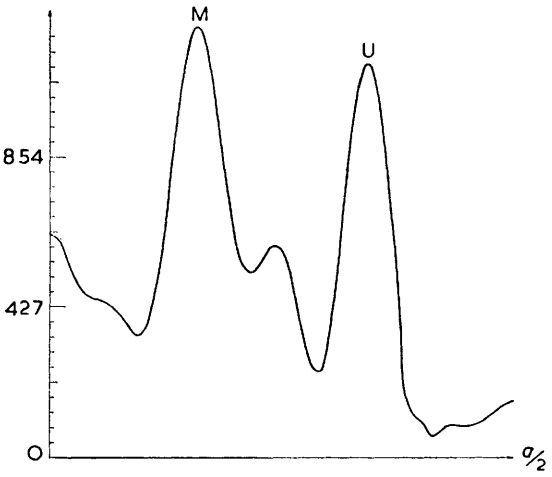


FIG. 1. *N*-5-Chlorosalicylideneaniline; generalised Patterson line synthesis $P_{k=1}(x,\frac{1}{2})$ in absolute units.

respectively. Rather than apply graphical corrections we chose the following analytical procedure: it was noted that M was surrounded by unmodified vectors due to *c*-glide plane related carbon atoms (1,2,3,5,7,8) while *U* was overlapped by unmodified vectors due to carbons 1 and 9, as well as by modified vectors due to the screw-axis related carbon atoms 1,2,3,5,7,8. (Vectors due to carbons 4,6,10,12,13, oxygen, and nitrogen fell outside the regions of U and M and could be ignored.) The carbon-vector contributions to the height of M, being independent of their y parameters, could be calculated from theoretical temperature-corrected carbon–carbon vector profiles (with temperature factors derived from the two-dimensional refinement); these were subtracted from the observed peak M to yield the " pure " modified peak M′. Since U contained y_C-dependent contributions which could not be allowed for at this stage, it was replaced by the theoretical profile U′ corrected by the chlorine temperature factor. Comparison of M′ and U′ yielded $y_{Cl} = \pm 0{\cdot}034$ (to be compared with the value of 0·0315 after refinement).

The value of $-0{\cdot}034$ was chosen arbitrarily. Next, the $(h0l)$ projection was fitted to a molecular model which suggested the essentially coplanar arrangement of the two benzene rings. The heights of the light atoms, relative to chlorine at $-0{\cdot}034$ were deduced from this model, and two sets of y co-ordinates calculated for the molecular orientations relative to the positive b direction. Rather than discriminate between the two sets of co-ordinates by structure-factor calculations we returned once more to the Patterson line synthesis. Since the (alternative) contributions of the modified carbon–carbon vectors, corresponding to the two sets of y_C-co-ordinates, could now be computed the observed peak height U, composed of U′, the y_C-independent carbon–carbon vectors, and either of the two modified carbon vector sets, provided a choice for the molecular orientation. The numerical computations indicated an acute molecular tilt

to the positive b direction; the corresponding co-ordinates were inserted into structure-factor calculations which confirmed the correctness of this choice.

Positions of the hydrogens attached to carbon were computed on the basis of C–H bond lengths of 1·08 Å and of normal bond angles. A series of thermally isotropic cycles, in which the hydrogen parameters were not allowed to move, was followed by anisotropic cycles in which the positional and isotropic thermal parameters of the hydrogens were also adjusted. Refinement was stopped when all residual shifts had been reduced to values equal or less than one tenth of the corresponding standard deviations. The refinement of the room-temperature data followed a strictly analogous procedure. The "final" agreement factors are: $r = \Sigma w(k^2F_o^2 - |F_c|^2)^2/\Sigma wk^4F_o^4 = 0{\cdot}014$; $R = \Sigma(|kF_o - |F_c||)/\Sigma kF_o = 0{\cdot}057$ for all reflections excepting $|F_c| < |kF_{threshold}|$; at low temperature, $r = 0{\cdot}023$; $R = 0{\cdot}062$.

Results

An electron-density projection $\rho(zx)$ of the room-temperature structure is shown in Fig. 2; two reflections, $F(200)$ and $F(203)$, believed to suffer from secondary extinction were included in the summation as F_c rather than F_o.

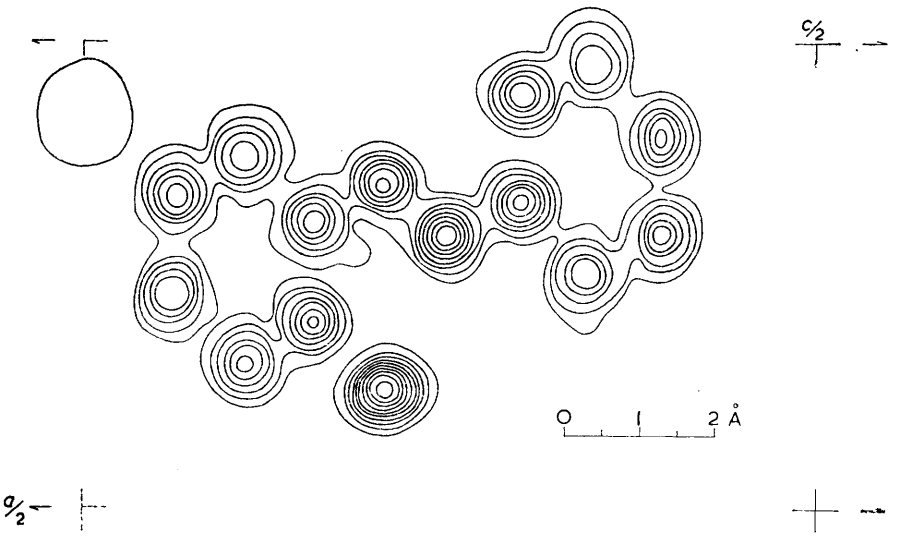


FIG. 2. *N*-5-Chlorosalicylideneaniline; electron-density projection $\rho(xz)$. Contour interval 1 e/Å²; lowest contour 2 e/Å². Contours on the chlorine atom are omitted.

TABLE 2.

Atomic co-ordinates (Å).

Atom	Low temperature			Room temperature			Atom	Low temperature			Room temperature		
	x	y	z	x	y	z		x	y	z	x	y	z
C_1	2·352	2·061	3·081	2·371	2·106	3·069	N	2·575	3·622	4·859	2·584	3·649	4·858
C_2	3·715	1·674	3·082	3·743	1·749	3·068	O	4·577	2·224	3·984	4·595	2·296	3·961
C_3	4·206	0·761	2·155	4·219	0·821	2·137	Cl	0·956	−0·141	0·000	0·966	−0·085	0·000
C_4	3·365	0·205	1·214	3·387	0·288	1·198							
C_5	2·011	0·564	1·207	2·025	0·632	1·202	H_3	5·176	0·504	2·209	5·232	0·648	2·177
C_6	1·500	1·468	2·123	1·526	1·504	2·118	H_4	3·651	−0·524	0·479	3·708	−0·496	0·575
							H_6	0·578	1·766	2·093	0·601	1·790	2·120
C_7	1·811	3·007	4·020	1·838	3·050	4·022	H_7	0·859	3·273	3·937	0·930	3·232	3·971
C_8	2·065	0·087	5·778	2·078	0·069	5·785	H_9	−0·047	0·060	5·211	0·024	−0·013	5·195
C_9	0·719	0·523	5·821	0·737	0·499	5·829	H_{10}	−0·608	1·744	6·846	−0·544	1·668	6·877
C_{10}	0·335	1·444	6·760	0·348	1·399	6·782	H_{11}	0·913	2·681	8·446	0·905	2·516	8·408
C_{11}	1·241	1·996	7·675	1·259	1·935	7·679	H_{12}	3·221	1·971	8·329	3·160	1·787	8·282
C_{12}	2·584	1·573	7·623	2·572	1·543	7·626	H_{13}	3·968	0·530	6·616	4·026	0·589	6·575
C_{13}	2·982	0·642	6·678	3·000	0·608	6·670							

To locate the hydrogen atom (not included at any stage in the least-squares calculations) in the O···N region we computed difference syntheses $\delta(xz)$ from $\Delta F(h0l)$ with phase angles of the three-dimensional refinement; these were followed by three-dimensional plane sections with $\Delta F(hkl)$ (Figs. 3 and 4) parallel to [010] whose x,z parameters corresponded to the maxima in $\delta(xz)$ in the O···N region. The peak in the low-temperature projection $\delta(xz)$ is fairly round with a height of 0·5 e/Å^2; the corresponding three-dimensional plane sections (Fig. 3) show a maximum of approximately 0·5 e/Å^3; the centre of this peak lies at 1·03 Å from the oxygen, such that the line joining this peak to the oxygen makes an angle of 104° with the O–C_2 bond; the peak lies 0·1 Å above the best plane defined by

TABLE 3.

Standard deviations (Å) of atomic co-ordinates.

Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	Atom	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
	Low temperature			Room temperature				Low temperature			Room temperature		
C_1	0·0047	0·0053	0·0044	0·0036	0·0046	0·0040	N	0·0036	0·0053	0·0033	0·0028	0·0036	0·0033
C_2	0·0042	0·0065	0·0041	0·0033	0·0049	0·0041	O	0·0029	0·0039	0·0034	0·0029	0·0036	0·0037
C_3	0·0039	0·0067	0·0043	0·0038	0·0051	0·0045	Cl	0·0015	0·0013		0·0010	0·0014	
C_4	0·0045	0·0059	0·0044	0·0041	0·0050	0·0045	H_3	0·046	0·083	0·062	0·040	0·050	0·051
C_5	0·0038	0·0072	0·0045	0·0038	0·0052	0·0041	H_4	0·065	0·094	0·064	0·041	0·054	0·050
C_6	0·0037	0·0064	0·0043	0·0033	0·0046	0·0039	H_6	0·057	0·087	0·062	0·033	0·041	0·037
C_7	0·0040	0·0065	0·0045	0·0037	0·0047	0·0040	H_7	0·071	0·087	0·079	0·054	0·060	0·063
C_8	0·0041	0·0058	0·0060	0·0039	0·0041	0·0042	H_9	0·046	0·059	0·050	0·074	0·055	0·057
C_9	0·0041	0·0069	0·0044	0·0040	0·0052	0·0047	H_{10}	0·082	0·102	0·084	0·056	0·061	0·067
C_{10}	0·0044	0·0062	0·0043	0·0046	0·0052	0·0051	H_{11}	0·066	0·097	0·085	0·068	0·060	0·085
C_{11}	0·0055	0·0064	0·0044	0·0054	0·0056	0·0046	H_{12}	0·050	0·053	0·053	0·047	0·046	0·052
C_{12}	0·0045	0·0068	0·0043	0·0050	0·0057	0·0047	H_{13}	0·073	0·111	0·089	0·055	0·069	0·065
C_{13}	0·0043	0·0067	0·0043	0·0047	0·0050	0·0046							

TABLE 4.

Thermal parameters (Å^2).

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}	Atom	U
				Low temperature				
C_1	0·0095	0·0068	0·0116	−0·0038	0·0054	0·0009	H_3	−0·014
C_2	0·0122	0·0085	0·0109	0·0002	0·0009	−0·0006	H_4	0·004
C_3	0·0143	0·0122	0·0103	0·0031	0·0024	0·0044	H_6	−0·009
C_4	0·0178	0·0039	0·0114	−0·0017	0·0029	0·0017	H_7	0·015
C_5	0·0099	0·0087	0·0102	−0·0006	−0·0034	−0·0006	H_9	−0·026
C_6	0·0114	0·0071	0·0149	0·0005	0·0017	−0·0015	H_{10}	0·015
C_7	0·0116	0·0062	0·0145	0·0003	−0·0002	−0·0001	H_{11}	0·008
C_8	0·0102	0·0090	0·0195	0·0003	−0·0009	−0·0005	H_{12}	−0·021
C_9	0·0099	0·0116	0·0133	0·0018	−0·0015	−0·0012	H_{13}	0·018
C_{10}	0·0150	0·0066	0·0149	0·0063	0·0015	0·0025		
C_{11}	0·0204	0·0154	0·0107	0·0009	0·0071	0·0056		
C_{12}	0·0179	0·0062	0·0118	−0·0004	0·0016	−0·0018		
C_{13}	0·0157	0·0067	0·0133	−0·0006	0·0054	−0·0017		
N	0·0100	0·0152	0·0082	0·0014	0·0035	0·0011		
O	0·0068	0·0129	0·0149	−0·0038	−0·0038	−0·0018		
Cl	0·0109	0·0145	0·0089	−0·0021	−0·0032	−0·0013		
				Room temperature				
C_1	0·0328	0·0396	0·0362	0·0013	0·0062	0·0039	H_3	0·012
C_2	0·0373	0·0402	0·0384	−0·0032	0·0028	−0·0002	H_4	0·018
C_3	0·0379	0·0533	0·0484	0·0098	−0·0020	0·0112	H_6	−0·007
C_4	0·0421	0·0535	0·0418	0·0036	−0·0030	0·0058	H_7	0·035
C_5	0·0381	0·0439	0·0366	−0·0063	−0·0016	−0·0032	H_9	0·032
C_6	0·0313	0·0410	0·0384	−0·0028	0·0007	−0·0023	H_{10}	0·038
C_7	0·0318	0·0361	0·0460	−0·0026	0·0072	0·0023	H_{11}	0·056
C_8	0·0402	0·0417	0·0391	−0·0011	0·0050	0·0053	H_{12}	0·016
C_9	0·0373	0·0388	0·0518	0·0039	0·0005	0·0032	H_{13}	0·042
C_{10}	0·0482	0·0475	0·0561	0·0096	0·0058	0·0120		
C_{11}	0·0688	0·0406	0·0432	0·0058	0·0012	0·0144		
C_{12}	0·0619	0·0504	0·0433	−0·0038	−0·0014	−0·0041		
C_{13}	0·0481	0·0404	0·0481	−0·0029	0·0044	−0·0035		
N	0·0297	0·0357	0·0386	0·0015	−0·0004	0·0011		
O	0·0279	0·0760	0·0572	0·0010	−0·0119	−0·0051		
Cl	0·0510	0·0629	0·0414	−0·0105	−0·0095	−0·0042		

TABLE 5.

Standard deviations (in Å²) of thermal parameters.

Atom	$\sigma(U_{11})$	$\sigma(U_{22})$	$\sigma(U_{33})$	$\sigma(U_{12})$	$\sigma(U_{23})$	$\sigma(U_{13})$	Atom	$\sigma(U)$
				Low temperature				
C_1	0·0016	0·0035	0·0017	0·0017	0·0019	0·0014	H_3	0·012
C_2	0·0016	0·0039	0·0016	0·0020	0·0022	0·0014	H_4	0·016
C_3	0·0016	0·0037	0·0017	0·0018	0·0022	0·0015	H_6	0·012
C_4	0·0019	0·0038	0·0016	0·0019	0·0019	0·0016	H_7	0·024
C_5	0·0015	0·0035	0·0016	0·0018	0·0021	0·0011	H_9	0·012
C_6	0·0016	0·0037	0·0016	0·0017	0·0021	0·0015	H_{10}	0·020
C_7	0·0015	0·0037	0·0017	0·0019	0·0022	0·0015	H_{11}	0·020
C_8	0·0019	0·0043	0·0024	0·0018	0·0021	0·0013	H_{12}	0·012
C_9	0·0014	0·0036	0·0017	0·0020	0·0022	0·0014	H_{13}	0·020
C_{10}	0·0016	0·0040	0·0017	0·0020	0·0021	0·0014		
C_{11}	0·0018	0·0039	0·0017	0·0023	0·0020	0·0017		
C_{12}	0·0018	0·0034	0·0015	0·0021	0·0020	0·0014		
C_{13}	0·0017	0·0034	0·0018	0·0020	0·0020	0·0014		
N	0·0012	0·0033	0·0013	0·0019	0·0016	0·0011		
O	0·0014	0·0031	0·0013	0·0013	0·0014	0·0012		
Cl	0·0004	0·0008	0·0004	0·0003	0·0006	0·0003		
				Room temperature				
C_1	0·0014	0·0028	0·0015	0·0029	0·0037	0·0027	H_3	0·010
C_2	0·0014	0·0026	0·0016	0·0031	0·0038	0·0028	H_4	0·012
C_3	0·0016	0·0031	0·0020	0·0034	0·0046	0·0033	H_6	0·007
C_4	0·0018	0·0030	0·0017	0·0038	0·0041	0·0032	H_7	0·016
C_5	0·0017	0·0027	0·0016	0·0033	0·0037	0·0026	H_9	0·015
C_6	0·0015	0·0026	0·0016	0·0030	0·0037	0·0029	H_{10}	0·014
C_7	0·0015	0·0027	0·0018	0·0031	0·0035	0·0029	H_{11}	0·021
C_8	0·0017	0·0030	0·0017	0·0034	0·0039	0·0028	H_{12}	0·010
C_9	0·0016	0·0025	0·0021	0·0034	0·0043	0·0030	H_{13}	0·016
C_{10}	0·0020	0·0031	0·0022	0·0041	0·0045	0·0037		
C_{11}	0·0024	0·0029	0·0019	0·0044	0·0041	0·0035		
C_{12}	0·0025	0·0033	0·0019	0·0046	0·0045	0·0035		
C_{13}	0·0019	0·0026	0·0019	0·0041	0·0041	0·0034		
N	0·0011	0·0021	0·0013	0·0026	0·0032	0·0022		
O	0·0012	0·0026	0·0016	0·0027	0·0031	0·0024		
Cl	0·0004	0·0007	0·0003	0·0009	0·0011	0·0009		

TABLE 6.

C–H bond lengths and angles.

Bond	Length (Å)	Angle			
		Low temperature			
C_3–H_3	1·00	C_2–C_3–H_3	118·2°	C_4–C_3–H_3	121·5°
C_4–H_4	1·07	C_3–C_4–H_4	125·3	C_5–C_4–H_4	115·3
C_6–H_6	0·97	C_5–C_6–H_6	122·1	C_1–C_6–H_6	117·8
C_7–H_7	0·99	C_1–C_7–H_7	118·9	N–C_7–H_7	119·6
C_9–H_9	1·08	C_8–C_9–H_9	121·6	C_{10}–C_9–H_9	118·3
C_{10}–H_{10}	0·99	C_9–C_{10}–H_{10}	121·9	C_{11}–C_{10}–H_{10}	116·0
C_{11}–H_{11}	1·08	C_{10}–C_{11}–H_{11}	121·2	C_{12}–C_{11}–H_{11}	120·3
C_{12}–H_{12}	1·03	C_{11}–C_{12}–H_{12}	116·6	C_{13}–C_{12}–H_{12}	123·3
C_{13}–H_{13}	0·99	C_{12}–C_{13}–H_{13}	113·8	C_8–C_{13}–H_{13}	124·4
		Room temperature			
C_3–H_3	1·03	C_2–C_3–H_3	114·9	C_4–C_3–H_3	124·2
C_4–H_4	1·05	C_3–C_4–H_4	120·9	C_5–C_4–H_4	118·7
C_6–H_6	0·97	C_5–C_6–H_6	122·8	C_1–C_6–H_6	116·5
C_7–H_7	0·93	C_1–C_7–H_7	116·9	N–C_7–H_7	121·3
C_9–H_9	1·08	C_8–C_9–H_9	117·7	C_{10}–C_9–H_9	122·2
C_{10}–H_{10}	0·94	C_9–C_{10}–H_{10}	122·1	C_{11}–C_{10}–H_{10}	116·7
C_{11}–H_{11}	1·00	C_{10}–C_{11}–H_{11}	117·7	C_{12}–C_{11}–H_{11}	122·3
C_{12}–H_{12}	0·91	C_{11}–C_{12}–H_{12}	120·8	C_{13}–C_{12}–H_{12}	118·1
C_{13}–H_{13}	1·03	C_{12}–C_{13}–H_{13}	112·3	C_8–C_{13}–H_{13}	126·6

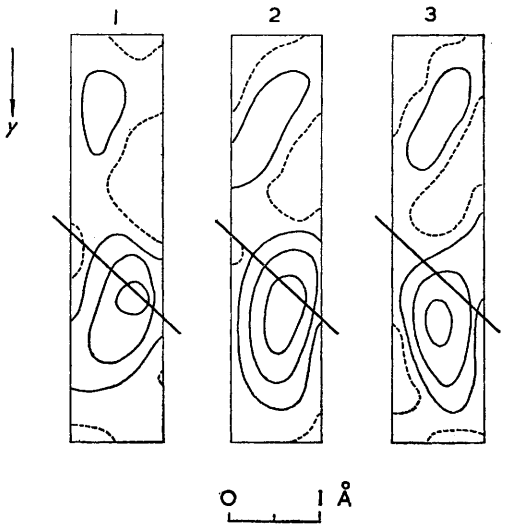


FIG. 3. *N*-5-Chlorosalicylideneaniline; parallel sections of $\delta(xyz)$ in the O · · · N region at low temperature. Contour interval 0·125 e/Å^3; zero contour dotted. The co-ordinates *xyz* of the upper left corners are: **1** (0·323, 0·134, 0·203); **2** (0·342, 0·134, 0·206); **3** (0·360, 0·134, 0·209). Distance between sections 0·2 Å. The trace of ring C is shown.

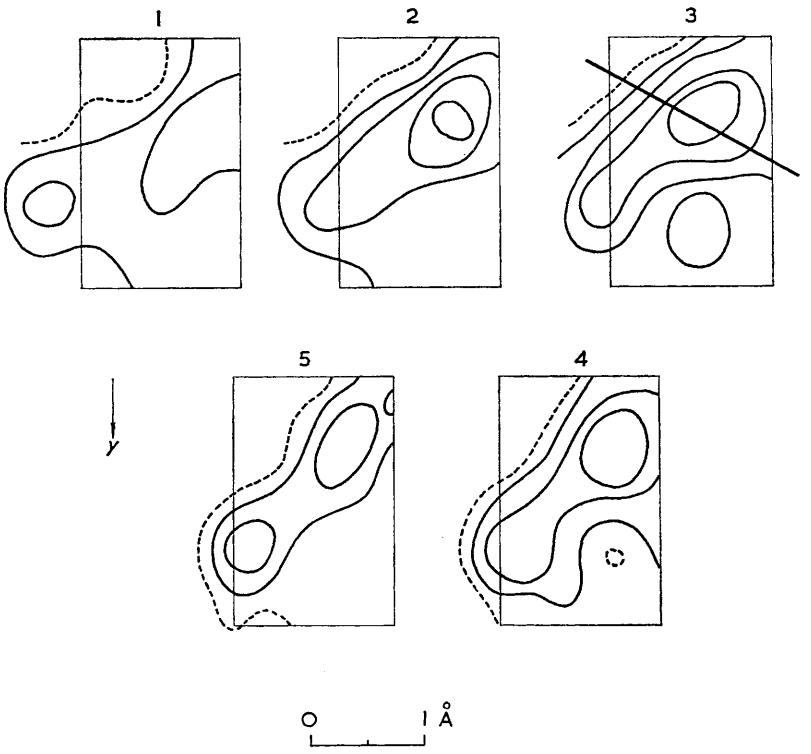


FIG. 4. *N*-5-Chlorosalicylideneaniline; parallel sections of $\delta(xyz)$ in the O · · · N region at room temperature. Contour interval 0·063 e/Å^3; zero contour dotted. The co-ordinates (*xyz*) of the upper left corners are **1** (0·305, 0·486, 0·179); **2** (0·293, 0·486, 0·185); **3** (0·281, 0·486, 0·192); **4** (0·267, 0·486, 0·198); **5** (0·255, 0·486, 0·204). Distance between sections 0·2 Å. The trace of ring C is shown in section **3** only.

TABLE 7.

(*a*) Equations of best planes.

		Low temperature				Room temperature			
		m_1	m_2	m_3	d	m_1	m_2	m_3	d
Ring A	$C_1 \cdots C_6$	2·4879	3·3533	−12·1438	0·0711	2·3929	3·4110	−12·2357	0·1116
Ring B	$C_8 \cdots C_{13}$	2·5057	3·2929	−12·4365	0·0576	2·4445	3·3608	−12·4655	0·1346
Ring C	O, C_2, C_1, C_7, N	2·4601	3·2504	−12·6676	−0·0703	2·3408	3·3246	−12·6934	−0·0109

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

(*b*) Deviations (Å) from best planes.

Atom	Low temperature Ring A	Low temperature Ring C	Room temperature Ring A	Room temperature Ring C
C_1	+0·007	+0·013	+0·008	+0·008
C_2	−0·004	+0·007	+0·006	+0·008
C_3	−0·002		−0·016	
C_4	+0·004		+0·011	
C_5	+0·000		+0·004	
C_6	−0·006		−0·013	
C_7	+0·013	−0·028	+0·018	−0·021
O	+0·015	−0·013	+0·023	−0·011
Cl	+0·018		+0·012	
N	+0·100	+0·021	+0·088	+0·016

Atom	Low temperature Ring B	Room temperature Ring B
C_8	−0·009	−0·012
C_9	+0·007	+0·013
C_{10}	−0·002	−0·006
C_{11}	−0·001	−0·001
C_{12}	−0·002	+0·002
C_{13}	+0·007	+0·005
N	−0·005	−0·022

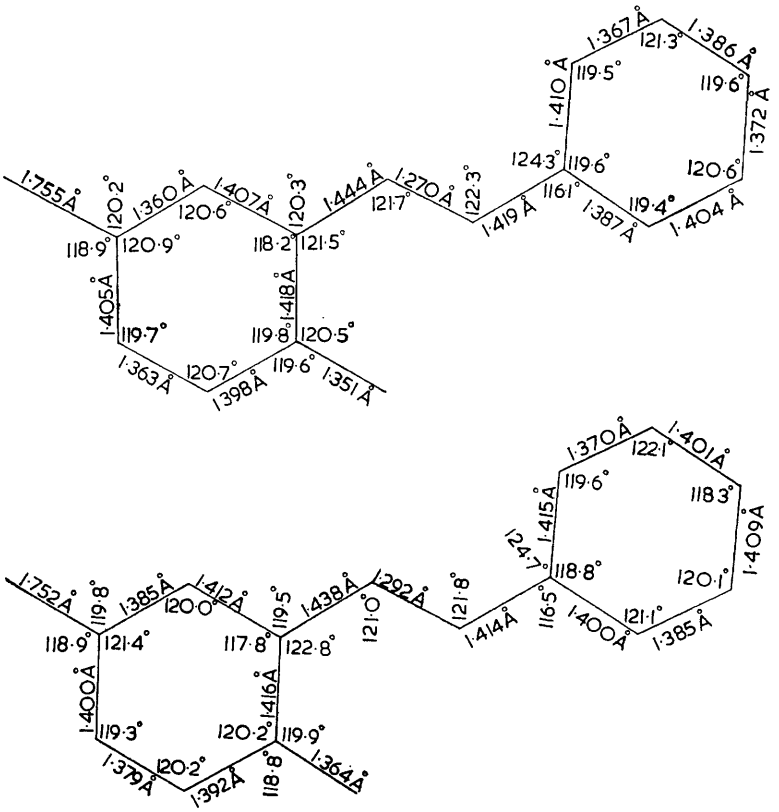


FIG. 5. *N*-5-Chlorosalicylideneaniline; experimentally determined bond lengths and bond angles at room temperature (top) and near 90°K (bottom).

TABLE 8.

Structure factors.

Low temperature data

h	k	l	$100kF_o$	$100A_c$	$100B_c$	$100F_c$
0	0	4	2421	−1366	2300	2675
		6	4927	3665	3281	4919
		8	3176	3046	−852	3163
		10	5454	5392	−34	5393
		12	2933	2516	−1361	2860
		14	4046	3553	−1506	3859
		16	1952	1886	−854	2071
		18	4088	4209	975	4320
		20	7277	6852	3942	7905
		22	3832	−2804	−2119	3514
		24	1253	1119	−349	1172
2	0	0	6024	−6651	0	6651
		1	5739	−6174	2140	6534
		2	5583	4003	−4342	5906
		3 *	8176	−1542	9384	9509
		4	4017	3872	448	3898
		5	3191	−1276	3028	3286
		6	5014	4378	−1861	4757
		7	5924	1461	5596	5784
		8	3645	2815	−2112	3519
		9	1936	1395	774	1595
		10	5198	4886	1604	5143
		11	1809	−238	1739	1755
		12	2492	−432	1963	2010
		13	4457	−785	4359	4429
		14	2279	2179	300	2199
		15	2463	743	2347	2461
		16	1482	1363	−391	1418
		17	3305	22	3549	3549
		18	<200	3	−33	33
		19	1696	1133	1255	1691
		20	1253	373	−1312	1364
		21	2308	−1614	971	1884
		22	3803	3468	−105	3470
		23	2835	−456	2650	2689
		24	1026	891	404	979
4	0	0	4302	−4213	0	4213
		1	4842	1145	4799	4934
		2	5755	−939	−5840	5915
		3	5454	−2858	5039	5793
		4	4357	−2122	3537	4125
		5	3532	2533	2616	3642
		7	4215	−1029	4240	4363
		8	1823	−328	1742	1772
		9	4814	319	4873	4883
		10	4247	−7677	−2426	8051
		11	3503	−782	3449	3536
		12	2848	2704	304	2721
		13	2036	224	2068	2080
		14	826	−759	504	911
		15	1509	−390	1442	1493
		16	1068	−993	−436	1084
		17	3162	480	3224	3259
		18	2379	−1896	1540	2443
		19	2107	−366	2091	2123
		20	1667	−824	−1428	1649
		21	2036	360	1850	1885
		22	456	−204	−349	404
		23	1909	−588	1610	1714
6	0	0	1865	−2051	0	2051
		1	4101	−3882	−1601	4199
		2	6367	−5081	3716	6295
		3	3975	3516	1619	3870
		4	3690	−3526	248	3535
		5	1923	325	1814	1843
		6	2848	−2713	−848	2842
		7	314	249	229	338
		8	4030	−4079	−29	4079
		9	1395	−587	1181	1319
		10	3091	−3041	−291	3055
		11	868	−425	774	883
		12	3460	−3526	−57	3527
		13	398	−236	299	381
		14	1952	−1878	712	2009
		15	456	−170	449	480
		16	2577	−2480	−853	2623
		17	754	−751	−5	751
		18	1780	−1646	−936	1893
		19	1923	1920	36	1920
		20	3004	−2307	1624	2822
		21	1097	−1085	−122	1092
		22	3033	−2849	533	2898
8	0	0	2777	−2446	0	2446
		1	628	−219	−616	653
		2	1838	−1914	−34	1914
		3	1580	363	−1397	1444
		4	2550	−2478	−926	2645
		5	3360	−471	−3299	3332
8	0	6	4001	−3303	2490	4136
		7	5454	−4073	−4377	5978
		8	4017	−1085	−4096	4237
		9	2648	1437	−2180	2611
		10	1751	−636	1780	1891
		11	1880	952	−1888	2114
		12	3832	−3324	2342	4066
		13	3561	3535	−1231	3743
		14	3205	−1067	−3168	3342
		15	2392	−1722	−1851	2528
		16	2308	−2211	1065	2454
		17	1553	−1186	−863	1466
		18	1026	−1020	0	1020
		19	770	−453	−656	797
		20	1467	−1529	−259	1551
		21	1438	−104	−1545	1549
10	0	0	512	484	0	484
		1	3574	429	−3895	3919
		2	770	755	206	783
		3	2635	−1099	−2480	2713
		4	2337	256	−2566	2579
		5	3004	1835	−2637	3213
		6	256	93	287	301
		7	3289	2812	−2000	3451
		8	3334	1906	3078	3621
		9	2877	−2643	−1063	2848
		10	1509	−585	−1497	1607
		11	1224	459	−1218	1302
		12	3091	2873	−1340	3170
		13	4428	−2634	−4069	4847
		14	1424	−1244	764	1460
		15	2820	418	−2564	2598
		16	1224	−395	1003	1078
		17	2250	1213	−1714	2099
		18	1110	906	−560	1065
12	0	0	912	815	0	815
		1	570	241	−564	613
		2	3075	3309	−901	3429
		3	1965	−1989	−648	2092
		4	2577	2133	1956	2894
		5	1197	428	−1189	1264
		6	2677	2619	−682	2707
		7	1197	856	−867	1218
		8	984	986	−197	1006
		9	1153	−524	−1088	1208
		10	1809	1788	−95	1790
		11	1068	694	−692	980
		12	1580	1457	−132	1463
		13	1282	−345	−1220	1268
		14	2877	2733	−90	2734
		15	599	405	−413	579
14	0	0	1936	1870	0	1870
		1	841	−564	635	849
		2	1794	1278	871	1546
		3	1894	861	1457	1692
		4	2906	2791	−488	2834
		5	3162	−10	2904	2904
		6	227	163	44	168
		7	1438	−1173	−446	1255
		8	1923	1982	106	1985
		9	955	341	865	930
		10	2023	2056	178	2064
0	1	2	6380	7406	−1591	7575
		4 *	10,980	9307	13,024	16,007
		6	5383	2975	−4348	5268
		8	2194	2236	−422	2276
		10	1936	1567	−821	1769
		12	2906	3018	−377	3042
		14	3432	3383	−119	3385
		16	6523	6297	−1999	6606
		18	2221	1195	2152	2462
		20	1809	1673	−331	1705
		22	2308	2086	1003	2315
		24	1696	1066	1578	1904
1	1	1	2933	−1497	−2682	3071
		2	2906	−2779	−641	2852
		3	3716	−2538	3230	4108
		4 *	7804	8717	−2702	9126
		5	2891	1702	−2571	3083
		6	1366	−804	978	1266
		7	997	−206	−1031	1051
		8	1253	940	−553	1091
		9	1324	153	−1292	1301
		10	654	−229	555	600
		11	527	61	−497	501
		12	797	360	688	777
		13	441	180	−441	476
		14	512	432	248	498
1	1	15	955	−113	−811	819
		16	1952	1295	1491	1974
		17	926	127	861	871
		18	2535	−2032	−1514	2534
		19	1197	596	−1141	1287
		20	854	−387	−760	853
		21	984	−540	−679	868
		22	1240	1204	146	1213
		23	783	−685	98	692
		24	1823	1943	623	2040
2	1	0	883	800	0	800
		1	4785	−1518	4871	5102
		2	1894	1351	1405	1949
		3	6865	5828	5288	7870
		4	5341	2379	−5069	5600
		5	3447	−1840	2967	3491
		6	4615	4241	−1961	4673
		7	4286	−3683	2439	4418
		8	3859	2382	2952	3793
		9	3817	1758	3150	3607
		10	3347	3337	−33	3337
		11	2635	−258	2675	2688
		12	2221	1964	−692	2083
		13	4117	2396	3353	4122
		14	2078	771	2026	2168
		15	1923	−600	1947	2038
		16	398	257	219	337
		17	2435	−1808	1663	2457
		18	2350	1689	−1558	2298
		19	2535	868	2453	2602
		20	868	878	−30	878
		21	2078	−124	1985	1989
		22	1625	1398	−297	1429
		23	2337	841	2061	2226
		24	1722	1845	−579	1933
3	1	0	171	87	0	87
		1	3489	−3687	−161	3690
		2	2292	2126	−895	2307
		3	3062	3074	−1037	3244
		4	2179	−268	−2019	2037
		5	1153	1112	−94	1116
		6	4215	2755	2680	3844
		7	741	−54	−728	730
		8	1068	−959	243	989
		9	2392	−1320	1844	2267
		10	699	−68	−666	669
		11	1097	492	743	891
		12	1295	945	−680	1164
		13	1211	121	−1020	1028
		14	2065	1974	−160	1981
		15	854	−533	−726	901
		16	1268	−762	1012	1267
		17	456	−216	−252	332
		18	1240	1247	110	1252
		19	1055	839	815	1170
		20	427	116	−381	398
		21	1010	−537	−743	917
		22	628	596	60	599
		23	1253	1087	408	1161
4	1	0	2107	2072	0	2072
		1	4885	236	5139	5145
		2	3803	−3650	988	3781
		3	3120	−298	3097	3111
		4	1696	−495	−1695	1766
		5	4331	674	4245	4298
		6	4671	−2629	3214	4153
		7	3405	−510	3233	3273
		8	2706	−2006	−1825	2712
		9	3191	395	3207	3231
		10	841	−86	690	695
		11	2719	−607	2612	2682
		12	1880	−2036	54	2036
		13	2848	27	2887	2887
		14	1767	−391	−1737	1781
		15	2463	−57	2353	2354
		16	2052	−1522	1498	2135
		17	1767	347	1906	1937
		18	797	−783	−379	870
		19	2208	−399	2538	2569
		20	712	−88	723	728
		21	1952	51	1799	1800
		22	1467	−1384	−271	1410
		23	1382	143	1477	1484
5	1	0 *	243	−187	0	187
		1	1509	1285	−808	1518
		2	4402	2248	3720	4347
		3	2719	−1353	2270	2643
		4	414	307	324	447

TABLE 8. (*Continued.*)

h	k	l	100kF_o	100A_c	100B_c	100F_c
5	1	5	2363	984	1974	2206
		6	2933	−1891	−2109	2833
		7	1467	−1325	−738	1517
		8	1767	1574	782	1758
		9	712	568	394	691
		10	485	351	−44	354
		11	498	−485	281	561
		12	770	702	167	722
		13	1211	1119	416	1194
		14	1395	−1455	33	1456
		15	1538	−1188	1130	1640
		16	1738	1610	−579	1711
		17	699	340	548	645
		18	1211	1292	−318	1331
		19	541	−116	−606	617
		20	1039	−546	771	945
		21	754	421	481	639
		22	1311	20	1313	1313
		23	1068	−900	815	1214
6	1	0	3476	−3305	0	3305
		1	754	541	−418	684
		2	2791	−2621	−963	2792
		3	1625	250	1569	1589
		4	3432	−3299	768	3387
		5	1738	326	−1547	1581
		6	5512	−5387	−737	5437
		7	3247	1259	3041	3291
		8	3532	−3055	835	3167
		9	1010	−533	897	1044
		10	1126	−970	152	982
		11	556	−379	518	642
		12	3574	−3585	−495	3619
		13	1467	−1425	461	1498
		14	3191	−3355	−211	3362
		15	1168	889	−832	1217
		16	1495	−1495	85	1497
		17	984	−291	995	1037
		18	2094	−2110	639	2205
		19	398	454	122	470
		20	2036	−2010	−274	2028
		21	456	166	428	459
		22	1538	−1584	119	1588
7	1	0	1068	−962	0	962
		1	1667	21	1610	1611
		2	556	−162	−463	491
		3	683	435	497	660
		4	570	89	−554	561
		5	1424	−1210	−378	1268
		6	1224	−1014	316	1062
		7	628	160	439	467
		8	1010	621	−771	990
		9	1667	−1651	−28	1651
		10	995	516	773	929
		11	3062	2741	1284	3027
		12	812	−391	611	726
		13	670	−609	192	639
		14	1010	−745	−693	1018
		15	541	470	324	571
		16	612	−292	588	657
		17	1097	−944	754	1208
		18	<185	−118	−30	122
		19	826	−80	753	757
		20	641	−276	−596	657
		21	641	−133	602	617
8	1	0	3489	−3607	0	3607
		1	2408	−465	−2183	2232
		2	1139	−900	353	967
		3	2007	−1849	−748	1995
		4	3703	−3733	−556	3774
		5	2677	−1079	−2260	2504
		6	670	−550	−352	653
		7	1809	−298	−1718	1744
		8	1625	−870	1285	1552
		9	4529	1622	−4447	4734
		10	4814	−4976	−1354	5157
		11	3075	−231	−3154	3163
		12	683	699	131	711
		13	314	266	125	293
		14	1965	−1907	556	1987
		15	854	474	−771	905
		16	2435	−2547	−307	2565
		17	712	−51	−647	649
		18	385	−350	−25	351
		19	2194	−469	−2124	2175
		20	1965	−1977	−282	1997
9	1	0	1509	−1347	0	1347
		1	<214	23	−132	134
		2	955	−688	688	973
		3	1780	−1510	−886	1751
		4	1909	45	−1972	1972
		5	1851	1637	975	1905
		6	527	−157	452	479
		7	1197	1190	66	1192
9	1	8	2550	−1836	1819	2584
		9	1353	143	1430	1437
		10	854	667	−623	913
		11	1838	−1911	209	1923
		12	1880	−790	−2004	2155
		13	1126	−649	−972	1169
		14	1026	−148	1030	1040
		15	343	−259	180	315
		16	1651	−982	1040	1431
		17	1923	1746	−127	1750
		18	1110	−32	−1054	1054
		19	470	−474	−44	477
10	1	0	1865	−2024	0	2024
		1	2693	293	−2708	2724
		2	754	746	108	754
		3	4486	1607	−4565	4840
		4	2392	2484	−82	2485
		5	541	319	−502	595
		6	427	−284	425	511
		7	2777	171	−2875	2880
		8	1809	991	−1572	1858
		9	1253	−643	−887	1096
		10	527	163	452	480
		11	1722	−262	−1712	1732
		12	1010	−54	1175	1176
		13	2791	−352	−3046	3066
		14	1197	942	−691	1168
		15	1909	−590	−1779	1874
		16	1567	1237	581	1367
		17	3803	380	−3695	3714
		18	955	−443	−797	912
11	1	0	456	−376	0	376
		1	<227	13	105	106
		2	485	−495	2	495
		3	912	518	−693	865
		4	1809	796	1710	1886
		5	1240	−1193	35	1194
		6	1282	−1070	−925	1415
		7	754	145	−783	796
		8	441	−379	−204	431
		9	485	100	−503	512
		10	955	−1006	−3	1006
		11	583	255	−611	662
		12	<185	−53	91	105
		13	485	380	−265	464
		14	683	−609	−220	648
		15	612	262	499	564
		16	1340	1237	−558	1357
		17	641	−448	−606	754
12	1	0	4386	4803	0	4803
		1	441	395	218	451
		2	1224	1234	504	1333
		3	1424	−25	−1452	1452
		4	1139	1210	−33	1210
		5	1224	−709	−936	1174
		6	2450	2618	310	2636
		7	1340	12	−1528	1528
		8	1240	1360	−444	1431
		9	512	256	−461	527
		10	2949	2711	105	2714
		11	699	−109	−681	690
		12	1153	1145	−21	1145
		13	1253	774	−952	1227
		14	2250	2284	−263	2299
		15	414	379	−226	442
13	1	0	612	−679	0	679
		1	1026	713	−808	1077
		2	770	666	350	753
		3	414	452	28	453
		4	427	−435	−330	547
		5	<185	−143	−157	212
		6	1055	152	−986	997
		7	968	−851	−52	853
		8	968	−208	907	930
		9	1809	−116	−1657	1661
		10	1936	1683	151	1690
		11	1395	1218	−473	1307
		12	955	−610	−641	885
		13	641	−70	667	671
14	1	0	2107	1976	0	1976
		1	1424	670	1144	1326
		2	1952	1748	438	1802
		3	1651	−549	1476	1574
		4	1495	1364	−105	1368
		5	414	264	281	385
		6	1224	1167	−95	1170
		7	1981	34	1863	1863
		8	1865	1849	366	1885
		9	826	−434	588	730
		10	1010	1069	−201	1088
15	1	0	1282	1251	0	1251
		1	470	436	8	436
		2	1068	−801	310	859
15	1	3	456	−76	−431	438
		5	683	−13	−600	601
0	2	2	3561	3520	540	3561
		4	4402	4417	−1022	4534
		6	5069	4332	872	4418
		8	2764	−924	2335	2511
		10	4642	4513	−1054	4634
		12	3176	1850	−2756	3319
		14	4615	4074	764	4145
		16	2165	1933	658	2042
		18	2648	2400	−182	2407
		20	2706	2039	439	2085
		22	1596	1600	−121	1605
1	2	0	683	725	0	725
		1	1153	378	−992	1062
		2	298	84	−263	276
		3	3318	2860	−1419	3193
		4	4159	−69	−4188	4188
		5	2308	−1770	−1356	2230
		6	912	268	−879	919
		7	3191	−2931	−691	3011
		8	5312	3504	3729	5117
		9	3218	1867	−2197	2883
		10	912	586	−593	834
		11	1880	167	−1815	1823
		12	2606	2436	−527	2492
		13	1994	1580	817	1779
		14	2693	−2026	1623	2596
		15	1268	−383	−1187	1248
		16	1055	−676	648	937
		17	1823	−972	−1435	1733
		18	1126	602	−988	1157
		19	314	215	−309	377
		20	912	847	−318	905
		21	754	388	−566	687
		22	812	556	−555	786
		23	754	574	−409	704
2	2	0	1453	1431	0	1431
		1	2194	1448	1674	2215
		2	1453	1145	−907	1461
		3	5127	−1903	4782	5147
		4	3460	3027	−1083	3215
		5	1696	1656	717	1804
		7	5924	−28	6320	6320
		8	3975	3866	−194	3871
		9	570	−103	353	368
		10	2521	2281	669	2377
		11	2052	556	1904	1984
		12	1936	1601	582	1703
		13	4188	−1384	3604	3861
		14	556	−117	−565	578
		15	654	414	569	703
		16	1894	1436	809	1648
		17	3191	431	3027	3057
		18	854	752	−364	835
		19	770	15	717	717
		20	1625	1318	−523	1418
		21	1952	386	1556	1603
		22	1438	1258	−284	1289
		23	1580	−467	1574	1642
3	2	0	670	659	0	659
		1	725	−41	−698	699
		2	3447	3191	−520	3233
		3	797	−811	−293	862
		4	2007	−396	1642	1689
		5	1453	−145	−1497	1504
		6	2292	1590	1418	2131
		7	4101	3165	2102	3799
		8	2933	1667	−2362	2891
		9	427	43	375	378
		10	570	306	296	426
		11	1738	−1718	−319	1747
		12	1952	1174	1388	1818
		13	2150	−2025	−412	2066
		14	2292	1755	−1575	2358
		15	1994	1963	−391	2002
		16	427	351	−127	373
		17	414	243	86	257
		18	2208	1497	1243	1946
		19	556	130	−399	419
		20	725	612	−187	640
		21	200	−189	70	202
		22	1353	1096	410	1170
4	2	0	3091	−2957	0	2957
		1	2820	461	2748	2786
		2	3020	1047	2527	2736
		3	3645	−162	3475	3479
		4	2635	−2000	1488	2493
		5	4871	−2436	4181	4839
		6	2735	−2732	−1851	2535
		7	2265	1638	1514	2230
		8	1295	−1155	161	1166
		9	2593	−131	2281	2285

TABLE 8. (*Continued.*)

h	*k*	*l*	100kF_o	100A_c	100B_c	100F_c
4	2	10	1851	−1640	−130	1645
		11	2265	397	1851	1893
		12	912	−922	264	959
		13	2337	−326	2069	2094
		14	1168	−1274	272	1303
		15	3859	833	3807	3897
		16	897	−3	−853	853
		17	1667	−455	1479	1547
		18	498	447	−135	467
		19	1823	46	1472	1473
		20	2279	−1997	563	2075
		21	1965	−6	1799	1799
		22	1366	−647	1173	1339
5	2	0	1609	1624	0	1624
		1	2577	636	2329	2414
		2	1667	1071	1200	1609
		3	1224	−1062	−48	1063
		4	1596	1079	−890	1399
		5	1068	737	579	937
		6	1738	−848	1487	1711
		7	1838	−634	1527	1653
		8	1311	1094	−492	1200
		9	1026	334	935	993
		10	968	886	−39	887
		11	1055	−447	817	931
		12	<243	99	40	107
		13	797	25	793	793
		14	968	611	−867	1061
		15	243	−198	232	305
		16	1324	912	779	1199
		17	1110	577	924	1089
		18	1110	980	−266	1016
		19	1567	−872	1076	1385
		20	883	341	703	781
		21	670	136	643	657
6	2	0	3334	−3240	0	3240
		1	1981	−643	1767	1881
		2	4144	−4016	−327	4029
		3	2648	1377	−2056	2475
		4	2279	−2077	522	2142
		5	1767	1046	1386	1736
		6	2279	−1580	−1311	2053
		7	1722	−1564	359	1605
		8	3247	−2907	978	3067
		9	2337	1355	1743	2208
		10	2978	−2651	−392	2680
		11	2078	−1866	528	1940
		12	2321	−2092	−84	2094
		13	1211	987	470	1094
		14	2550	−2044	1307	2427
		15	1082	−1028	−291	1068
		16	2078	−2098	−472	2150
		17	1240	695	−836	1087
		18	2991	−2504	−125	2507
		19	1880	−267	1669	1690
		20	1823	−1764	−219	1777
		21	272	45	291	294
7	2	0	683	−655	0	655
		1	1082	−429	937	1031
		2	1353	−1110	−764	1347
		3	1224	195	1147	1164
		4	1359	−1042	−722	1267
		5	4101	−2123	3123	3777
		6	2194	1990	725	2118
		7	955	778	−518	935
		8	<243	143	−173	225
		9	683	107	−650	658
		10	3205	−3007	−545	3056
		11	654	641	196	670
		12	1596	1303	930	1601
		13	1596	80	1631	1633
		14	628	588	216	626
		15	3120	43	3034	3034
		16	2136	−1761	−51	1762
		17	441	−334	−121	356
		18	641	−615	−52	617
		19	527	−191	457	496
		20	441	−30	−430	431
8	2	0	2107	−1930	0	1930
		1	1240	−722	−953	1195
		2	2094	−2087	−129	2091
		3	1495	156	−1425	1433
		4	1311	−396	−1161	1227
		5	3817	−1276	−3455	3683
		6	3518	−2900	1808	3417
		7	1366	370	−1254	1307
		8	2107	−1891	−636	1995
		9	2179	113	−1946	1950
		10	1197	−1059	235	1085
		11	1709	65	−1697	1698
		12	2078	−1961	−206	1972
		13	1324	−7	−1237	1237
		14	1838	−1147	−1174	1641
8	2	15	2535	1216	−1657	2056
		16	2065	−1087	1424	1791
		17	1382	−1086	−729	1308
		18	1838	−1623	−371	1665
		19	1139	−261	−1011	1044
9	2	0	3276	−3077	0	3077
		1	2036	1942	43	1943
		2	783	−152	−683	700
		3	826	473	−726	866
		4	1324	−486	1223	1316
		5	1495	1403	353	1447
		6	1567	−1359	−811	1582
		7	498	−297	355	462
		8	1482	−998	−887	1335
		9	2292	−1315	1843	2264
		10	570	−431	292	521
		11	1139	228	1258	1278
		12	1738	−1592	746	1758
		13	1182	−306	−1104	1146
		14	641	−586	−102	595
		15	1282	−865	−777	1163
		16	812	132	−740	751
		17	683	379	−396	548
10	2	0	1524	1412	0	1412
		1	4215	2727	−2806	3913
		2	912	579	665	882
		3	2363	−254	−2200	2214
		4	1110	−594	−886	1067
		5	2094	181	−2020	2028
		6	1097	893	509	1028
		7	1382	222	−1265	1284
		8	369	288	−14	289
		9	2435	−575	−2239	2311
		10	770	749	−86	754
		11	2250	348	−1924	1955
		12	385	269	−82	281
		13	2179	−804	−1768	1943
		14	741	628	−339	714
		15	2052	66	−1851	1852
		16	712	−598	24	598
		17	1865	25	−1951	1951
11	2	0	4130	4104	0	4104
		1	343	−307	226	381
		2	1680	−1674	139	1679
		3	1182	−975	−786	1252
		4	2379	−2199	619	2285
		5	1153	−270	−1150	1182
		6	628	−598	163	619
		7	897	575	−740	937
		8	385	−373	−199	422
		9	1253	−440	−1059	1147
		10	654	−543	−30	543
		11	955	708	−338	784
		12	485	−436	−265	510
		13	812	−187	−725	748
		14	912	−721	−461	856
		15	612	661	−354	750
12	2	0	2150	1974	0	1974
		1	1126	−728	−505	886
		2	2463	1733	−1022	2012
		3	1253	−140	−1110	1119
		4	2606	1835	1047	2112
		5	556	−388	15	388
		6	2065	1209	−1203	1770
		7	783	−213	−619	655
		8	3104	2565	755	2674
		9	2308	505	−1824	1893
		10	1880	1554	−193	1566
		11	1495	431	−1193	1268
		12	2265	2026	−75	2027
		13	272	5	302	302
13	2	0	628	−647	0	647
		1	1438	−586	−1138	1280
		2	485	−98	−436	447
		3	256	21	−225	226
		4	599	550	−148	569
		5	485	6	−490	490
		6	984	831	−228	862
		7	1794	−66	−1501	1503
		8	641	−502	1	502
		9	441	227	−297	374
		10	1068	952	262	988
14	2	0	398	421	0	421
		1	1110	−510	966	1093
		2	2479	2215	95	2217
		3	926	458	750	878
		4	1353	1114	575	1254
		5	955	−375	836	917
		7	1139	779	907	1195
0	3	2	3376	3502	−881	3611
		4	1253	1182	419	1254
		6	2835	2834	−231	2844
		8	2036	2102	434	2146
0	3	10	3218	3080	−492	3119
		12	1482	1282	−557	1398
		14	2521	2369	589	2441
		16	1366	1212	−320	1253
		18	2236	2222	159	2228
		20	1424	1422	−403	1478
1	3	0	3289	−3506	0	3506
		1	2107	−1163	−1924	2248
		2	1580	1410	−478	1489
		3	628	−41	−697	698
		4	1751	1694	−455	1754
		5	1596	−204	−1623	1636
		6	1153	1051	−618	1219
		7	968	214	−850	876
		8	2036	1746	−1172	2103
		9	2308	956	−2201	2400
		10	2007	1679	1133	2026
		11	2065	−653	−1925	2032
		12	1923	−345	1866	1898
		13	<398	−20	−387	387
		14	<398	321	−43	324
		15	1055	486	−987	1100
		16	699	681	69	684
		17	654	−37	−752	752
		18	599	−142	−540	559
		19	1395	580	−1249	1377
		20	1153	−552	−940	1090
		21	1224	−493	−1279	1371
2	3	0	2150	2187	0	2187
		1	3262	−2212	2598	3412
		2	654	591	−337	681
		3	939	496	823	961
		4	1311	1077	740	1307
		5	2350	628	2180	2269
		6	1981	2038	176	2045
		7	1197	1087	486	1191
		8	3360	2942	−2041	3580
		9	5370	1533	5440	5651
		10	1596	−1632	178	1641
		11	4402	−4089	1894	4506
		12	3389	2504	2550	3574
		13	1268	1297	−315	1335
		14	1509	1331	−997	1664
		15	1538	−14	1603	1603
		16	968	736	−750	1051
		17	1211	719	1016	1245
		18	541	517	127	532
		19	2208	229	2067	2080
		20	1097	1129	109	1135
3	3	0	2492	2487	0	2487
		1	699	682	−9	682
		2	1936	1828	981	2074
		3	583	334	−465	573
		4	1324	1350	112	1355
		5	683	357	−456	579
		6	1794	1751	447	1807
		7	441	−383	79	391
		8	1524	1443	−251	1464
		9	612	171	373	410
		10	883	−654	−479	811
		11	570	−232	153	278
		12	2479	2499	439	2537
		13	398	165	−153	225
		14	1609	1739	−189	1749
		15	527	−76	−640	644
		16	1153	1236	25	1237
		17	<327	21	−312	312
		18	1596	1608	63	1609
		19	<256	−182	222	287
		20	1097	949	506	1076
4	3	0	327	−3	0	3
		1	3532	−153	3698	3701
		2	327	−32	202	204
		3	1295	−169	1208	1220
		4	1696	−1539	−614	1657
		5	2408	130	2395	2399
		6	2221	−1413	1769	2264
		7	1340	−855	1115	1405
		8	1553	−1550	438	1610
		9	2421	−2254	851	2410
		10	754	−302	−529	609
		11	4586	4113	2842	4999
		12	1495	−1203	−1023	1580
		13	1625	−167	1636	1644
		14	712	−254	−768	809
		15	1625	−314	1748	1776
		16	939	−731	773	1064
		17	1638	−63	1724	1725
		18	<285	8	498	498
		19	2308	−471	2356	2402
		20	583	−553	463	721
5	3	0	356	312	0	313
		1	1625	−136	1536	1542

TABLE 8. (*Continued.*)

h	k	l	100kF_o	100A_c	100B_c	100F_c
5	3	2	1295	1248	467	1333
		3	1295	786	909	1202
		4	1082	982	−525	1114
		5	997	−396	908	990
		6	1126	893	433	992
		7	1353	129	1355	1361
		8	841	847	230	877
		9	1823	−562	1546	1645
		10	699	509	−234	561
		11	1268	90	1242	1245
		12	797	856	−29	856
		13	854	−169	835	852
		14	939	1041	127	1049
		15	556	69	631	634
		16	456	433	297	525
		17	683	−381	627	733
		18	868	856	−140	867
		19	1082	75	1130	1133
6	3	0	883	−903	0	903
		1	3476	2843	−2245	3623
		2	4985	−4278	−2370	4891
		3	3318	−1513	3069	3422
		4	1738	−1683	−20	1683
		5	1153	614	934	1130
		6	741	−662	262	712
		7	854	343	762	835
		8	2392	−2327	−250	2341
		9	699	−382	−526	650
		10	1651	−1403	485	1484
		11	<398	238	281	368
		12	2150	−2086	439	2132
		13	826	−588	641	870
		14	926	−781	382	870
		15	1110	−467	798	925
		16	2891	−2783	174	2789
		17	770	72	822	825
		18	2635	−2865	318	2883
7	3	0	1010	−1032	0	1032
		1	2450	625	2355	2437
		2	1324	57	−1287	1289
		3	1295	−848	908	1242
		4	754	−735	−233	771
		5	1268	−603	1069	1227
		6	1609	−1084	1032	1496
			854	−583	588	828

h	k	l	100kF_o	100A_c	100B_c	100F_c
7	3	8	699	231	−739	774
		9	926	226	931	958
		10	470	−183	463	498
		11	1253	534	1231	1342
		12	628	−488	483	687
		13	1126	761	1005	1260
		14	1382	−615	−1139	1294
		15	1596	−188	1558	1569
		16	897	−702	665	967
		17	1224	−279	1228	1259
		18	583	−267	572	631
8	3	0	1680	−1650	0	1650
		1	2621	−2359	−1102	2604
		2	1366	−796	1095	1355
		3	1609	710	−1379	1551
		4	1709	−1405	951	1696
		5	1965	354	−1930	1962
		6	2479	−2132	−1184	2438
		7	1722	16	−1828	1828
		8	997	−874	300	924
		9	712	−548	−267	609
		10	1567	−1587	−190	1599
		11	797	128	−829	839
		12	984	−983	108	989
		13	2007	145	−2016	2021
		14	1851	−1998	396	2037
		15	1709	−438	−1575	1635
		16	725	−195	−746	771
		17	385	−127	−423	442
9	3	0	<398	−45	0	45
		1	883	567	−724	919
		2	1767	−1791	495	1858
		3	<398	144	−253	291
		4	1894	−1849	−747	1994
		5	1680	473	1614	1682
		6	897	−870	−296	919
		7	1211	1211	742	1420
		8	1340	−894	1022	1358
		9	868	−941	470	1052
		10	1311	−1289	−574	1411
		11	556	−224	397	4563
		12	770	−554	−659	861
		13	1580	−1531	−309	1562
		14	1638	−1465	615	1589
		15	512	−28	509	509

h	k	l	100kF_o	100A_c	100B_c	100F_c
10	3	0	599	741	0	741
		1	1680	−1060	−1462	1806
		2	1182	1257	−71	1259
		3	2350	−746	−2589	2694
		4	1553	−1118	1135	1593
		5	1110	957	−628	1145
		6	783	498	−697	857
		7	2435	−72	−2601	2602
		8	398	445	−106	458
		9	1010	221	−1082	1104
		10	<298	195	−59	204
		11	1609	−767	−1516	1699
		12	298	259	71	269
		13	2078	342	−1888	1919
11	3	0	826	−885	0	885
		1	414	49	−434	436
		2	1182	−706	−490	859
		3	1126	−735	−737	1041
		4	1609	−542	1477	1574
		5	812	−477	−675	826
		6	527	−565	−278	630
		7	1197	63	−1101	1103
		8	1709	−1506	−949	1780
		9	1467	284	−1427	1455
		10	498	−457	196	497
		11	1110	341	−957	1016
		12	1282	−1466	282	1492
12	3	0	725	849	0	849
		1	1153	314	−1169	1210
		2	343	−354	−106	370
		3	1211	179	1253	1265
		4	3732	3882	−973	4002
		5	1722	−378	−1691	1733
		6	1580	1601	−140	1607
		7	1295	−416	−1227	1296
		8	683	637	356	730
		9	414	−234	−431	491
13	3	0	356	396	0	396
		1	897	−87	−930	934
		2	441	−300	40	303
		3	897	329	−975	1029
		4	414	558	19	558
		5	868	155	−1079	1090

Room temperature data

0	0	2	3774	−2685	3205	4181
		4	2943	−1438	2921	3256
		6	4856	3861	3139	4976
		8	2711	2739	−550	2794
		10	4509	4574	−454	4596
		12	2228	1782	−1130	2109
		14	2565	2216	−922	2400
		16	1388	1333	−342	1377
		18	2659	2779	318	2797
		20	3994	3816	1103	3972
		22	1975	−1779	108	1783
		24	557	496	−113	509
2	0	0*	5233	−6758	0	6758
		1*	5381	−6467	2148	6814
		2	5403	3949	−4546	6021
		3*	7787	−1236	9278	9360
		4	3669	3811	331	3825
		5	2953	−1245	4945	3198
		6	4225	3888	−1846	4304
		7	5097	1864	4754	5107
		8	2847	2464	−1727	3009
		9	946	756	560	941
		10	4352	4207	1001	4325
		11	1672	−569	1525	1628
		12	2092	−85	2028	2030
		13	3552	−44	3462	3462
		14	1493	1530	11	1530
		15	1545	503	1419	1505
		16	841	830	−238	864
		17	2154	293	2113	2133
		18	284	37	256	259
		19	683	299	621	689
		20	442	−16	−507	507
		21	1335	−1104	723	1320
		22	1829	1606	−392	1653
		23	1072	187	1013	1030
		24	410	347	206	404
4	0	0	3972	−4143	0	4143
		1	4352	990	4607	4713
		2	5128	−889	−5376	5450
		3	4792	−2564	4604	5270
		4	3898	−1634	3418	3788
		5	3143	2202	2092	3037

4	0	7	3826	−864	3652	3753
		8	1345	−244	1256	1279
		9	4120	449	3946	3971
		10	6358	−6380	−866	6439
		11	2795	−738	2728	2826
		12	2228	2158	−433	2201
		13	1324	70	1244	1246
		14	588	−503	373	626
		15	1113	−432	1051	1136
		16	819	−764	−122	773
		17	1713	435	1602	1660
		18	1020	−711	771	1049
		19	1135	−266	1197	1226
		20	903	−671	−616	911
		21	831	280	775	824
		22	<158	−111	−88	141
		23	778	−311	668	736
		24	483	−177	507	537
6	0	0	1061	−1099	0	1099
		1	3857	−3445	−1553	3779
		2	5444	−4345	3322	5470
		3	3499	3263	1319	3519
		4	2806	−2899	−130	2902
		5	1713	261	1717	1737
		6	2575	−2408	−636	2491
		7	<148	18	130	131
		8	2953	−3066	12	3066
		9	1051	−604	870	1059
		10	1987	−1972	−139	1977
		11	736	−197	631	661
		12	2407	−2334	−19	2334
		13	410	−267	218	345
		14	989	−922	341	983
		15	220	−32	240	242
		16	1576	−1639	−393	1685
		17	588	−625	73	629
		18	1008	−985	−421	1071
		19	810	753	−330	822
		20	1082	−573	759	951
		21	504	−425	254	495
		22	1177	−1136	244	1162
		23	578	383	599	711
8	0	0	2312	−2007	0	2007

8	0	1	399	−130	−376	397
		2	1156	−1272	57	1273
		3	1125	−7	−975	975
		4	1755	−1671	−714	1817
		5	2417	−500	−2344	2397
		6	2847	−2003	1865	2737
		7	3826	−2923	−2452	3815
		8	3311	−1353	−3009	3299
		9	2250	1094	−1867	2164
		10	1104	−22	1121	1121
		11	1335	589	−1247	1379
		12	2448	−1730	1565	2333
		13	2228	1986	−944	2199
		14	2396	−994	−2133	2353
		15	1177	−1137	−578	1275
		16	936	−745	598	955
		17	410	−399	−121	417
		18	399	−365	12	365
		19	305	−115	−288	310
		20	662	−740	−177	761
		21	588	−168	−623	646
10	0	0	168	57	0	57
		1	2386	393	−2326	2359
		2	494	447	136	467
		3	1598	−778	−1413	1613
		4	1629	−8	−1628	1628
		5	2269	1140	−1906	2221
		6	284	236	1	236
		7	2228	1908	−1190	2249
		8	2375	1513	1789	2343
		9	1576	−1498	62	1499
		10	1166	−871	−861	1225
		11	652	316	−521	609
		12	1808	1624	−1022	1919
		13	2365	−1615	−1892	2488
		14	1030	−720	784	1064
		15	1366	252	−1248	1273
		16	442	−19	376	376
		17	1051	642	−760	995
		18	525	232	−433	492
		19	704	70	−755	758
12	0	0	273	75	0	75
		1	210	134	−194	236

TABLE 8. (*Continued.*)

h	k	l	100kF_o	100A_c	100B_c	100F_c
12	0	2	1849	1836	−640	1945
		3	998	−989	−324	1041
		4	1576	1023	1236	1605
		5	516	186	−494	528
		6	1135	1118	−431	1198
		7	631	462	−473	661
		8	232	195	−61	204
		9	525	−292	−460	545
		10	967	868	27	868
		11	640	381	−445	586
		12	463	426	−190	467
		13	410	−115	−360	377
		14	1094	1055	−142	1064
		15	325	321	−68	329
		16	568	575	−212	613
14	0	0	956	909	0	909
		1	315	−234	153	280
		2	547	212	445	493
		3	862	615	442	757
		4	1376	1238	−334	1283
		5	1450	114	1332	1336
		6	315	−79	243	255
		7	989	−853	−278	898
		8	662	637	−90	644
		9	315	278	197	341
		10	736	708	85	713
		11	337	187	268	327
0	1	2	6989	6830	−2344	7221
		4*	10,552	9771	11,890	15,390
		6	4309	2197	−3764	4358
		8	1691	1695	−351	1731
		10	1481	1412	−168	1422
		12	2281	2321	−374	2351
		14	2701	2617	−284	2632
		16	3741	3392	−1636	3766
		18	1796	893	1652	1878
		20	841	827	−201	851
		22	1146	1046	266	1079
		24	946	736	654	985
1	1	0*	5276	−6416	0	6416
		1	3069	−1678	−2343	2882
		2	3605	−3348	−382	3369
		3	4068	−2447	3522	4288
		4*	7820	8086	−3353	8754
		5	2565	1661	−1881	2509
		6	1240	−492	1046	1156
		7	714	−156	−708	725
		8	946	662	−527	847
		9	967	190	−931	950
		10	778	−247	631	678
		11	200	62	−159	171
		12	819	296	736	793
		13	220	201	−195	280
		14	325	298	213	366
		15	294	64	−261	269
		16	1041	775	661	1019
		17	673	378	551	668
		18	1586	−1563	−422	1619
		19	588	120	−578	590
		20	273	−212	−289	359
		21	337	−281	−127	308
		22	599	576	−157	597
		23	200	−119	101	156
		24	778	781	−4	781
2	1	0	1082	1012	0	1012
		1	4572	−1545	4615	4867
		2	1954	1202	1555	1966
		3	6884	5465	4697	7206
		4	4908	1966	−4636	5036
		5	2995	−1739	2685	3199
		6	3984	3823	−1702	4185
		7	3984	−3230	2727	4227
		8	3511	2399	2545	3497
		9	2974	1618	2323	2831
		10	2544	2478	−313	2498
		11	2133	−108	2203	2206
		12	1503	1371	−458	1446
		13	2775	1689	2031	2641
		14	1796	960	1489	1771
		15	1388	−515	1332	1428
		16	241	95	269	285
		17	1861	−1047	1515	1842
		18	1166	711	−962	1196
		19	1125	612	957	1136
		20	504	530	154	552
		21	925	−10	935	935
		22	631	552	−133	568
		23	788	305	674	740
		24	662	576	−322	660
3	1	0	358	−333	0	333
		1	3143	−3422	87	3423
		2	1608	1549	−535	1639
		3	2974	2982	−942	3127
3	1	4	1713	−439	−1557	1617
		5	925	843	−172	860
		6	3311	2363	2290	3291
		7	483	−76	−467	474
		8	1450	−1328	337	1370
		9	2197	−934	1883	2101
		10	504	−263	−354	441
		11	810	568	471	738
		12	640	411	−471	625
		13	788	−105	−685	693
		14	1209	1167	−253	1194
		15	568	−480	−358	598
		16	956	−375	924	997
		17	241	−97	−100	139
		18	547	542	−115	554
		19	662	587	307	662
		20	<220	−98	−78	125
		21	284	240	−134	275
		22	<220	177	140	226
		23	483	461	42	463
		24	126	64	147	160
4	1	0	2260	2176	0	2176
		1	4309	331	4500	4512
		2	3268	−3099	975	3249
		3	2816	−419	2914	2944
		4	1608	−833	−1398	1627
		5	3373	540	3430	3472
		6	3531	−1919	2868	3451
		7	3026	−464	2860	2898
		8	2427	−1782	−1534	2351
		9	2427	262	2406	2421
		10	547	19	473	473
		11	2207	−355	2024	2054
		12	1481	−1349	313	1385
		13	1913	−46	1872	1873
		14	1440	−737	−1219	1425
		15	1586	−87	1512	1515
		16	1113	−563	948	1103
		17	883	160	947	960
		18	337	−383	−127	403
		19	1177	−151	1285	1294
		20	210	42	172	177
		21	810	86	749	754
		22	631	−576	87	583
		23	525	−47	528	531
5	1	0	568	−512	0	512
		1	1703	1409	−1007	1732
		2	3721	1923	3143	3685
		3	2269	−1087	1953	2235
		4	494	−209	438	485
		5	1755	1076	1366	1739
		6	2785	−1978	−1606	2548
		7	1567	−1384	−610	1513
		8	1376	1209	518	1315
		9	389	333	137	360
		10	220	92	−3	92
		11	420	−380	166	415
		12	399	410	44	413
		13	736	705	65	708
		14	1051	−986	317	1035
		15	998	−689	765	1030
		16	831	681	−512	852
		17	<241	154	80	174
		18	463	461	−87	469
		19	410	−301	−348	460
		20	640	−148	540	560
		21	<220	250	150	292
		22	452	73	443	449
		23	473	−236	410	473
6	1	0	3153	−3093	0	3093
		1	588	328	−375	498
		2	2250	−2056	−846	2223
		3	1471	258	1384	1408
		4	2711	−2534	794	2656
		5	1314	146	−1223	1232
		6	4151	−4151	−569	4190
		7	2522	1089	2206	2461
		8	2176	−1946	585	2032
		9	967	−547	698	887
		10	736	−725	−200	752
		11	337	−263	244	359
		12	2448	−2407	−40	2407
		13	967	−901	452	1008
		14	1934	−1919	139	1924
		15	525	224	−500	548
		16	704	−671	−224	708
		17	547	−29	563	564
		18	1051	−1012	435	1101
		19	<210	166	13	166
		20	967	−936	−183	954
		21	<200	−63	129	143
		22	599	−613	−1	613
7	1	0	915	−853	0	853
		1	1283	−105	1252	1257
		2	568	−231	−459	514
		3	200	213	56	220
		4	568	235	−432	492
		5	1376	−1174	−542	1293
		6	893	−793	213	821
		7	220	121	96	154
		8	640	356	−494	609
		9	1166	−1122	−113	1127
		10	609	285	548	617
		11	1944	1928	256	1945
		12	389	−187	296	350
		13	578	−578	84	584
		14	693	−586	−334	674
		15	<241	237	62	245
		16	232	−37	245	248
		17	631	−464	502	684
		18	<210	−64	−29	70
		19	<232	−22	255	256
		20	315	−227	−224	319
		21	<168	−187	128	227
		22	<115	−7	−78	78
8	1	0	2627	−2565	0	2565
		1	1576	−396	−1437	1491
		2	640	−512	165	538
		3	1240	−1069	−427	1151
		4	2701	−2748	−398	2777
		5	1913	−890	−1567	1802
		6	368	−211	−263	338
		7	1271	−251	−1254	1279
		8	1061	−426	852	953
		9	2859	824	−2802	2921
		10	3394	−3389	−616	3444
		11	1567	−406	−1544	1596
		12	673	518	−453	688
		13	494	541	20	541
		14	819	−781	356	858
		15	516	185	−493	527
		16	1199	−1320	39	1321
		17	210	−40	−280	283
		18	273	−41	−309	312
		19	915	−411	−789	890
		20	736	−748	1	748
		21	535	−352	−450	571
9	1	0	819	−803	0	803
		1	<232	−18	−207	207
		2	494	−293	376	477
		3	1251	−964	−790	1246
		4	1419	−59	−1466	1467
		5	1251	1244	367	1297
		6	378	222	373	434
		7	714	712	−154	729
		8	1493	−931	1158	1486
		9	1051	258	1020	1052
		10	778	545	−609	818
		11	1314	−1299	228	1319
		12	1187	−631	−1044	1220
		13	841	−502	−678	844
		14	535	217	512	556
		15	<220	−99	−26	103
		16	704	−340	540	638
		17	925	773	−390	866
		18	599	−90	−563	570
		19	168	−221	16	222
		20	126	−127	−11	127
10	1	0	1104	−1248	0	1248
		1	1555	−1	−1594	1594
		2	389	421	−27	422
		3	2838	942	−2819	2972
		4	1503	1535	−318	1567
		5	430	426	6	426
		6	631	−400	521	657
		7	1650	66	−1663	1664
		8	1356	451	−1222	1303
		9	599	−309	−380	489
		10	535	357	413	546
		11	746	−68	−762	765
		12	609	−7	626	626
		13	1397	−315	−1382	1418
		14	609	248	−564	617
		15	704	−240	−596	642
		16	621	586	141	602
		17	1586	51	−1489	1490
		18	535	−399	−241	466
		19*	358	198	−407	453
11	1	0	<253	103	0	103
		1	<241	48	19	51
		2	<241	−167	28	169
		3	494	318	−347	471
		4	1187	728	983	1223
		5	757	−703	265	752
		6	810	−678	−515	851
		7	420	−27	−407	408

TABLE 8. (*Continued.*)

h	*k*	*l*	100kF_o	100A_c	100B_c	100F_c
11	1	8	<241	−51	−122	132
		9	368	91	−387	397
		10	420	−406	−1	406
		11	442	141	−464	485
		12	<210	189	−21	190
		13	<241	236	−7	236
		14	263	−273	−100	290
		15	389	217	321	387
		16	726	616	−391	729
		17	253	−213	−207	297
12	1	0	2480	2613	0	2613
		1	241	324	114	343
		2	652	476	481	677
		3	673	−123	−653	664
		4	410	352	−35	354
		5	547	−361	−382	525
		6	1240	1302	42	1303
		7	693	1	−698	698
		8	442	406	−169	439
		9	294	130	−257	288
		10	1292	1184	−46	1185
		11	273	133	−274	304
		12	337	359	66	365
		13	557	294	−426	517
		14	851	725	−143	739
		15	284	279	−57	285
13	1	0	346	−376	0	376
		1	463	413	−342	536
		2	430	450	161	478
		3	368	316	199	373
		4	210	−258	−86	272
		5	<210	−79	−43	90
		6	516	179	−487	519
		7	504	−414	181	452
		8	483	4	404	404
		9	714	−154	−684	702
		10	714	706	−67	709
		11	798	724	−182	746
		12	399	−345	−134	370
		13	442	−5	454	454
14	1	0	683	636	0	636
		1	473	369	297	474
		2	788	685	118	695
		3	736	−323	664	739
		4	452	432	40	434
		5	210	157	−65	170
		6	420	355	−120	375
		7	757	196	723	750
		8	757	711	234	749
		9	315	−194	180	265
		10	210	183	−75	197
15	1	0*	599	552	0	552
		1	<168	202	119	234
		2	547	−442	143	465
		3	158	−173	−79	190
		4	389	354	−203	408
		5	284	19	−248	248
		6	<126	63	−9	63
0	2	2	3079	2847	465	2885
		4	3583	3711	−1054	3858
		6	4194	4353	18	4353
		8	2448	−373	2519	2546
		10	3332	3136	−1201	3358
		12	2007	1078	−1565	1900
		14	2859	2747	677	2829
		16	1156	1068	193	1085
		18	1030	1077	−99	1082
		20	1094	976	14	976
		22	578	585	−26	585
1	2	0	253	260	0	260
		1	693	524	−273	591
		2	420	−81	−364	373
		3	2618	2507	−680	2598
		4	3583	−634	−3467	3524
		5	1691	−1297	−817	1533
		6	893	−211	−788	815
		7	2386	−2275	62	2276
		8	4161	3347	2708	4305
		9	1902	1319	−1370	1902
		10	463	167	−304	347
		11	1020	362	−900	970
		12	1356	1268	−430	1339
		13	1471	1334	521	1432
		14	1913	−1232	1626	2040
		15	599	−367	−443	575
		16	621	−450	333	560
		17	621	−470	−342	581
		18	621	129	−557	572
		19	284	306	−38	308
		20	420	293	−176	342
		21	358	281	−190	339
		22	232	41	−165	170
		23	263	271	−111	293

h	*k*	*l*	100kF_o	100A_c	100B_c	100F_c
2	2	0	1345	1331	0	1331
		1	2154	1174	1565	1957
		2	1524	1277	−672	1443
		3	4141	−1384	4013	4245
		4	2880	2754	−765	2859
		5	1471	1259	248	1283
		6	494	−445	132	465
		7	4844	259	5030	5037
		8	2764	2898	−288	2913
		9	578	−168	531	557
		10	1839	1787	382	1827
		11	1376	96	1433	1437
		12	1113	1016	275	1052
		13	2480	−442	2405	2445
		14	358	−189	−169	253
		15	<253	−9	164	164
		16	1230	1195	396	1259
		17	1534	421	1467	1526
		18	452	380	−124	400
		19	389	−35	415	417
		20	621	494	−271	563
		21	736	107	717	725
		22	516	494	−57	497
		23	621	−7	647	647
3	2	0	253	284	0	284
		1	578	−246	−477	537
		2	2637	2483	−553	2544
		3	557	−600	43	601
		4	2081	−1024	1650	1942
		5	915	−213	−899	924
		6	1261	652	1101	1280
		7	3017	2588	1343	2915
		8	1787	761	−1566	1741
		9	430	19	360	361
		10	452	16	460	461
		11	1187	−1201	101	1205
		12	1051	649	805	1034
		13	1240	−1179	3	1179
		14	1094	331	−949	1005
		15	1156	1100	−373	1161
		16	<253	1	156	156
		17	<241	172	134	218
		18	1082	935	619	1121
		19	<220	35	−212	215
		20	<241	94	108	144
		21	<220	−62	189	199
		22	358	300	176	348
4	2	0	2260	−2143	0	2143
		1	2260	56	2309	2310
		2	2439	837	2173	2329
		3	2795	125	2663	2666
		4	2049	−1584	1092	1924
		5	3815	−1889	3491	3969
		6	1870	−1448	−1169	1861
		7	1598	1174	962	1517
		8	862	−817	−2	817
		9	1734	−176	1649	1659
		10	1113	−998	139	1007
		11	1335	202	1221	1238
		12	609	−592	131	606
		13	1461	−208	1410	1426
		14	631	−603	167	625
		15	2092	731	2048	2174
		16	504	−229	−455	509
		17	746	−362	725	811
		18	284	184	−185	261
		19	746	−117	692	702
		20	1041	−689	634	936
		21	714	28	685	686
		22	399	−144	335	365
5	2	0	631	633	0	633
		1	1503	308	1375	1409
		2	1187	413	1017	1098
		3	1166	−1028	−365	1091
		4	1113	501	−941	1066
		5	946	779	504	927
		6	1503	−743	1337	1530
		7	1051	−503	925	1054
		8	516	324	−395	511
		9	442	185	387	429
		10	378	327	−76	335
		11	609	−454	386	596
		12	253	−225	188	293
		13	253	−100	226	248
		14	253	162	−304	345
		15	253	−318	124	341
		16	652	547	479	727
		17	442	347	241	422
		18	<220	38	−120	126
		19	599	−318	455	555
		20	378	21	347	348
		21	<179	−84	49	98
		22	<126	−38	119	125

h	*k*	*l*	100kF_o	100A_c	100B_c	100F_c
6	2	0	2448	−2465	0	2465
		1	1555	−371	1434	1481
		2	3110	−2992	−248	3002
		3	1755	710	−1466	1629
		4	1409	−1407	−28	1408
		5	1082	618	892	1085
		6	1335	−1118	−947	1465
		7	1314	−1278	405	1341
		8	2102	−1860	971	2098
		9	1481	1118	923	1450
		10	1555	−1547	−200	1560
		11	1199	−1173	452	1257
		12	1251	−1309	−117	1314
		13	621	588	128	601
		14	1218	−892	756	1169
		15	578	−606	−16	606
		16	1156	−1170	−204	1187
		17	358	135	−305	334
		18	1230	−1174	54	1176
		19	841	−31	762	762
		20	673	−608	−86	614
		21	<148	−37	86	94
7	2	0	452	−436	0	436
		1	483	−254	373	451
		2	1061	−940	−447	1041
		3	516	20	508	508
		4	841	−599	−540	806
		5	2448	−1563	1762	2356
		6	1440	1395	412	1454
		7	1125	437	−1007	1097
		8	<253	−98	−14	99
		9	714	−187	−623	651
		10	1892	−1893	−111	1897
		11	253	275	−91	290
		12	810	764	182	785
		13	714	161	679	698
		14	241	218	14	218
		15	1125	272	1169	1200
		16	798	−787	211	815
		17	568	−477	−144	499
		18	325	−301	−107	320
		19	200	−241	60	248
		20	294	−56	−246	252
8	2	0	1335	−1309	0	1309
		1	893	−492	−729	879
		2	1283	−1296	−197	1311
		3	883	124	−862	871
		4	757	−243	−676	719
		5	2396	−821	−2147	2298
		6	2269	−1840	1314	2261
		7	621	504	−364	621
		8	1166	−1038	−545	1172
		9	1209	−66	−1199	1201
		10	621	−628	−17	629
		11	862	−109	−816	823
		12	1082	−962	−2	962
		13	588	−265	−534	596
		14	1030	−756	−700	1030
		15	1030	455	−939	1043
		16	662	−212	530	571
		17	473	−397	−124	416
		18	746	−726	−32	727
		19	494	7	−486	486
9	2	0	1787	−1837	0	1837
		1	1199	1259	−379	1315
		2	504	283	−379	473
		3	652	118	−592	604
		4	788	−89	782	787
		5	1041	1052	−47	1053
		6	977	−760	−689	1026
		7	253	−113	206	235
		8	767	−384	−627	735
		9	1113	−749	866	1144
		10	305	183	178	255
		11	452	201	422	468
		12	662	−566	460	729
		13	621	−418	−597	729
		14	<263	−202	−135	243
		15	778	−554	−440	708
		16	599	60	−589	592
		17	368	175	−332	375
		18	368	−353	120	373
10	2	0	568	657	0	657
		1	2176	1693	−1552	2297
		2	726	456	662	804
		3	1072	−177	−1093	1108
		4	810	−618	−496	793
		5	893	−36	−958	959
		6	662	633	117	643
		7	704	134	−651	665
		8	241	73	−91	116
		9	1113	−304	−1091	1133
		10	232	215	−151	263

TABLE 8. (*Continued.*)

h	*k*	*l*	100kF_o	100A_c	100B_c	100F_c
10	2	11	946	220	−956	981
		12	<220	125	−73	145
		13	819	−254	−646	694
		14	232	251	−65	259
		15	652	22	−609	609
		16	325	−243	−26	244
		17	673	−17	−668	669
11	2	0	2427	2546	0	2546
		1	253	−79	291	301
		2	746	−729	265	775
		3	631	−498	−378	625
		4	851	−815	386	902
		5	621	−193	−553	585
		6	<241	−93	−93	131
		7	410	179	−397	436
		8	<232	61	−130	144
		9	516	−230	−400	461
		10	<263	−63	15	65
		11	547	423	−201	468
		12	325	−0	−257	257
		13	662	25	−265	266
		14	210	−229	−136	266
		15	368	334	−201	389
12	2	0	746	806	0	806
		1	399	−378	−82	387
		2	946	646	−636	907
		3	640	38	−641	643
		4	936	881	567	1048
		5	273	−158	115	195
		6	746	335	−554	648
		7	516	−155	−433	460
		8	1261	1191	221	1212
		9	862	222	−718	751
		10	525	431	−54	434
		11	504	169	−468	497
		12	673	630	−51	632
		13	284	234	174	292
13	2	0	284	−289	0	289
		1	516	−408	−330	525
		2	346	55	−319	324
		3	<241	76	60	97
		4	410	300	−38	374
		5	<232	24	−7	25
		6	494	450	−36	452
		7	568	66	−543	547
		8	346	−258	193	322
		9	315	271	153	311
		10	547	481	−47	483
		11	<136	−133	−71	151
14	2	0	<189	18	0	18
		1	430	−266	331	424
		2	862	804	−45	805
		3	683	236	121	266
		4	325	319	138	348
		6	599	621	135	636
		7	483	415	273	497
		8	263	238	−155	284
0	3	2	2448	2312	−1045	2538
		4	967	878	−89	882
		6	1902	1970	−190	1979
		8	1629	1650	164	1658
		10	2407	2627	−204	2635
		12	337	321	8	321
		14	1292	1351	222	1370
		16	420	459	−64	463
		18	1072	903	−75	906
		20	726	630	−203	662
1	3	0	2764	−2771	0	2771
		1	1335	−1023	−818	1309
		2	1072	961	−202	982
		3	241	53	−227	233
		4	1041	919	−372	991
		5	683	−153	−618	637
		6	430	360	−291	463
		7	494	493	−116	506
		8	1094	724	−790	1072
		9	1218	783	−1005	1274
		10	1314	1209	606	1352
		11	915	−711	−687	989
		12	1366	−313	1332	1368
		13	263	188	103	215
		14	<210	−14	−69	71
		15	578	462	−352	581
		16	284	265	46	269
		17	232	131	−189	230
		18	294	−228	−19	229
		19	535	288	−341	447
		20	494	−349	−231	418
		21	241	−167	−220	276
2	3	0	1975	1964	0	1964
		1	2448	−1539	1785	2357
		2	494	483	109	496
		3	746	138	737	750
2	3	4	1051	883	598	1067
		5	1545	567	1493	1597
		6	1271	1288	231	1308
		7	831	730	549	913
		8	1902	1584	−1224	2002
		9	2995	1288	3031	3293
		10	1030	−987	317	1037
		11	2806	−2502	1469	2901
		12	1892	1808	887	2014
		13	494	458	−258	526
		14	673	467	−569	736
		15	788	117	771	780
		16	410	363	−283	461
		17	714	396	544	673
		18	410	381	106	396
		19	767	219	708	741
		20	557	503	113	516
		21	463	−235	401	465
3	3	0	1440	1348	0	1348
		1	767	654	206	686
		2	1283	653	961	1162
		3	305	119	−196	230
		4	578	521	191	555
		5	253	175	−206	271
		6	1061	968	431	1060
		7	535	−364	397	539
		8	420	332	−285	437
		9	253	194	−69	206
		10	1051	−1067	68	1070
		11	210	−1	133	133
		12	1218	1254	376	1310
		13	263	214	173	275
		14	621	654	−183	679
		15	200	−85	−203	220
		16	325	355	100	369
		17	<220	16	14	21
		18	442	380	45	382
		19	148	−99	140	172
		20	473	262	366	450
		21	210	241	44	245
4	3	0	525	−477	0	477
		1	2439	−111	2438	2440
		2	241	154	18	155
		3	925	−143	854	865
		4	1061	−1002	−225	1027
		5	1619	78	1627	1629
		6	1187	−665	979	1183
		7	1020	−346	924	987
		8	936	−897	338	959
		9	1703	−1431	738	1610
		10	726	−435	−383	579
		11	2375	2432	1159	2694
		12	757	−595	−420	728
		13	1061	−318	1001	1050
		14	200	−106	−183	211
		15	893	−105	942	947
		16	452	−90	404	414
		17	925	−34	790	791
		18	<189	−70	171	184
		19	893	−42	926	927
		20	378	−351	116	369
5	3	0	473	−473	0	473
		1	841	317	712	779
		2	473	447	114	462
		3	746	678	391	783
		4	599	209	−540	579
		5	609	−537	182	567
		6	525	263	383	465
		7	578	91	600	607
		8	420	349	208	406
		9	1051	−507	867	1004
		10	<210	−67	60	90
		11	452	116	490	504
		12	210	264	−57	270
		13	325	−191	200	277
		14	337	310	208	374
		15	189	−46	44	63
		16	253	−96	294	309
		17	463	−403	190	445
		18	<168	80	7	80
		19	337	47	311	314
		20	179	−38	193	197
6	3	0	767	−793	0	793
		1	2081	1773	−1098	2086
		2	3026	−2699	−1371	3027
		3	2164	−954	1976	2194
		4	915	−875	50	876
		5	525	251	467	530
		6	420	−352	−41	355
		7	368	−3	235	235
		8	1356	−1369	−57	1370
		9	452	−164	−298	340
		10	662	−599	306	673
6	3	11	210	−29	169	171
		12	1104	−1139	280	1173
		13	463	−44	446	448
		14	399	−425	169	457
		15	483	−138	424	446
		16	1199	−1108	169	1121
		17	305	−14	257	257
		18	977	−980	214	1003
		19	578	−238	−567	615
7	3	0	504	−531	0	531
		1	1104	303	1094	1135
		2	936	140	−946	957
		3	767	−713	−135	725
		4	640	−603	155	623
		5	494	−242	414	480
		6	946	−610	669	905
		7	368	−370	23	370
		8	599	38	−576	577
		9	<210	133	107	171
		10	210	−132	228	263
		11	200	92	211	231
		12	273	−193	270	332
		13	189	175	200	266
		14	788	−432	−583	725
		15	504	−220	413	468
		16	346	−257	229	344
		17	284	−44	272	276
		18	189	19	232	232
8	3	0	631	−629	0	629
		1	1524	−1466	−650	1604
		2	883	−514	831	977
		3	1146	752	−903	1175
		4	883	−804	399	897
		5	977	171	−928	944
		6	1356	−1284	−642	1435
		7	704	−13	−768	768
		8	410	−414	10	414
		9	200	−225	134	262
		10	851	−785	−5	785
		11	358	−129	−320	345
		12	442	−375	89	386
		13	883	−98	−853	858
		14	831	−831	159	846
		15	778	−324	−666	741
		16	516	−220	−423	477
		17	210	−55	−240	246
9	3	0	420	470	0	470
		1	662	301	−596	667
		2	726	−740	381	832
		3	389	160	−383	415
		4	915	−825	−401	917
		5	693	184	670	694
		6	346	−125	−250	279
		7	525	533	−41	535
		8	389	−86	413	422
		9	442	−454	154	479
		10	714	−516	−393	649
		11	<210	−114	71	134
		12	430	−34	−341	343
		13	810	−626	−302	695
		14	557	−393	266	475
		15	<136	40	104	112
10	3	0	<200	129	0	129
		1	599	−391	−496	631
		2	662	717	−120	726
		3	1209	−437	−1204	1281
		4	778	−610	533	811
		5	557	408	−411	579
		6	294	115	−304	325
		7	1304	−200	−1098	1116
		8	220	83	−82	117
		9	547	99	−555	563
		10	<200	178	−20	179
		11	578	−193	−567	599
		12	<168	41	−147	153
		13	831	161	−706	724
		14	253	−48	−222	227
11	3	0	<220	−143	0	143
		1	<220	107	−143	178
		2	557	−114	−492	505
		3	452	−420	−177	456
		4	652	77	598	603
		5	294	−186	−155	242
		6	<200	132	−42	138
		7	494	31	−470	471
		8	757	−505	−444	673
		9	631	43	−612	613
		10	158	152	95	179
		11	410	203	−373	425
		12	399	−398	93	409
12	3	0	325	351	0	351
		1	673	225	−598	639

TABLE 8. (*Continued.*)

h	*k*	*l*	100kF_o	100A_c	100B_c	100F_c	*h*	*k*	*l*	100kF_o	100A_c	100B_c	100F_c	*h*	*k*	*l*	100kF_o	100A_c	100B_c	100F_c
12	3	2	389	−314	−157	351	12	3	8	389	193	289	348	13	3	3	136	121	−182	219
		3	640	−55	604	607			9	158	28	−197	199			4	378	376	54	380
		4	1777	1577	−564	1675			10	430	483	−67	488			5	315	219	−247	330
		5	831	−184	−711	734	13	3	0	305	326	0	326			6	179	140	−151	206
		6	494	537	69	541			1	168	−42	−192	196							
		7	420	−19	−372	372			2	<136	−134	26	136							

O, carbons 2, 1, 7, and N (ring C). It is reasonable to interpret this peak as the hydroxylic hydrogen since the O–H length and the COH angle compare well with the corresponding values in salicyclic acid [9] (1·04 Å, 109°).

The electron-density distribution in the room-temperature structure is more diffuse; $\delta(xz)$ shows an elongated peak of maximum height 0·25 e/Å^2 which in the three-dimensional plane sections (Fig. 4) is resolved into two peak systems. The first, M_1 (>0·25 e/Å^3) lies at 0·89 Å from the oxygen, and in the plane of ring C such that the angle C_2OM_1 is 106·5°. The second peak, M_2 (<0·25 e/Å^3) lies at 1·65 Å from the oxygen, at an angle C_2OM_2 of 85°, and approximately 1 Å above ring C. M_1 may be assigned to the hydroxylic hydrogen; the meaning to be attached to M_2 is highly problematical.

One may not unjustifiably query the significance of these electron-density determinations on the grounds of inadequate experimental measurements (*e.g.*, photographic as well as only partial *hkl* data) and possibly incomplete refinement (diagonal approximation of the least-squares procedure used here). However, we have chosen to submit these findings on the grounds that they represent our experimental results, that the observed " hydrogen " positions are not unreasonable as regards bond lengths and angles, that they are partly confirmed by similar results of our analysis of 2-chloro-*N*-salicylideneaniline (Part X, following Paper) and by our partial refinement [10] of the structure of 5-chlorosalicylaldoxime.[11]

The positional and thermal parameters derived from the two sets of data, and their standard deviations estimated according to Part V [5] are listed in Tables 2—5. Bond lengths and bond angles are given in Figs. 5a and b; the C–H bond lengths and angles are found in Table 6. The best planes of the three rings C_1–C_6 (A), C_8–C_{13} (B), and $OC_2C_1C_7N$ (C) were computed according to Schomaker *et al.*[12] Table 7 lists their equations, as well as the distances of the substituent and ring atoms from these planes. Table 8 contains *hkl*, 100 kF_o, 100 A_c, 100B_c, and 100F_c. Reflections to which zero weight was attached are asterisked; all unobserved reflections are marked $<kF_o$.

Analysis of Thermal Vibrations.—The anisotropic thermal parameters obtained from the least-squares refinement were analysed for the translational and librational components of rigid-body motion by Cruickshank's method,[13] modified by Hirshfeld [14] for molecules in which the point of intersection of the axes of libration is not known. The magnitudes and direction cosines, with respect to the unit-cell axes, of the principal axes of the ellipsoids of motion are given in Table 9 which also lists the co-ordinates of the centre of libration. The ellipsoids of libration of the low-temperature and room-temperature structures agree closely both in the orientation and relative magnitudes of their respective principal axes. (The weakest principal component of libration of the low-temperature structure is negative; however, its magnitude is negligible.) The dominant mode of libration occurs about an axis lying along the length of the molecule; the molecule oscillates about an axis nearly normal to its plane. Its translational motion is almost isotropic.

The r.m.s. discrepancy of the rigid-body analysis equals $[\Sigma\Delta u_{ij}^2/(n-s)]^{\frac{1}{2}}$, where n is the total number of thermal parameters and s the number of independent parameters,

[9] Cochran, *Acta Cryst.*, 1953, **6**, 260.
[10] Leiserowitz and Schmidt, to be published.
[11] Simonsen, Pfluger, and Thompson, *Acta Cryst.*, 1961, **14**, 269.
[12] Schomaker, Waser, Marsh, and Bergman, *Acta Cryst.*, 1959, **12**, 600.
[13] Cruickshank, *Acta Cryst.*, 1956, **9**, 754, 757.
[14] Hirshfeld, Sandler, and Schmidt, *J.*, 1963, 2108.

TABLE 9.

Principal components of rigid-body vibrations and their direction cosines relative to the crystal axes. Co-ordinates of centres of libration.

	Low temperature				Room temperature		
	a	*b*	*c*		*a*	*b*	
$T_1^2 = 0.0094$ Å^2 ...	−0·9845	0·1601	−0·0719	$T_1^2 = 0.0266$ Å^2 ...	−0·9555	−0·1955	0·2211
$T_2^2 = 0.0078$	0·1749	0·9286	0·3273	$T_2^2 = 0.0440$	−0·0146	−0·7168	−0·6971
$T_3^2 = 0.0125$	0·0143	−0·3348	−0·9422	$T_3^2 = 0.0326$	0·2948	−0·6693	0·6820
$\omega_1^2 = -0.00008$ rad.^{2}	−0·9908	−0·0147	−0·1345	$\omega_1^2 = 0.00028$ rad.^{2}	−0·9808	0·0352	−0·1916
$\omega_2^2 = 0.00028$	0·0599	0·8434	−0·5340	$\omega_2^2 = 0.00131$	0·1478	0·7752	−0·6143
$\omega_3^2 = 0.00139$	0·1213	−0·5371	−0·8347	$\omega_3^2 = 0.00738$	0·1269	−0·6308	−0·7655
Libration centre at	*x*	*y*	*z*				
Low temperature...	2·671	2·624	3·800				
Room temperature	2·237	2·758	3·719				

i.e., six translational, six librational, and three defining the origin of libration. The r.m.s. discrepancy equals 0·0028 and 0·0042 Å^2 for the low-temperature and room-temperature structures, respectively. The corresponding r.m.s. standard deviations of thermal vibration from the least-squares procedure are 0·0021 and 0·0028 Å^2. Because the least-squares estimate is likely to be too small the differences between the two sets of r.m.s. values cannot be regarded as evidence for internal vibrations.

Table 10 shows that the agreement between the observed and calculated thermal

TABLE 10.

Thermal parameters (Å^2) derived from the analysis of rigid-body motion.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{23}	U_{13}
			Low temperature			
C_1	0·0096	0·0085	0·0120	−0·0004	0·0014	0·0000
C_2	0·0100	0·0092	0·0124	0·0003	0·0012	0·0001
C_3	0·0116	0·0099	0·0127	0·0012	0·0011	0·0005
C_4	0·0133	0·0079	0·0117	0·0001	0·0020	0·0007
C_5	0·0125	0·0090	0·0122	−0·0012	0·0012	0·0000
C_6	0·0105	0·0103	0·0129	−0·0008	0·0005	−0·0004
C_7	0·0095	0·0091	0·0124	0·0000	0·0012	0·0000
C_8	0·0119	0·0082	0·0118	0·0000	0·0018	0·0005
C_9	0·0130	0·0109	0·0132	0·0022	0·0009	0·0006
C_{10}	0·0163	0·0114	0·0134	0·0035	0·0011	0·0013
C_{11}	0·0191	0·0079	0·0115	0·0015	0·0026	0·0018
C_{12}	0·0174	0·0075	0·0113	−0·0011	0·0023	0·0010
C_{13}	0·0137	0·0083	0·0118	−0·0012	0·0016	0·0003
N	0·0100	0·0083	0·0119	−0·0003	0·0015	0·0001
O	0·0096	0·0123	0·0140	0·0007	−0·0003	−0·0005
Cl	0·0156	0·0127	0·0141	−0·0026	−0·0007	−0·0011
			Room temperature			
C_1	0·0281	0·0380	0·0377	−0·0010	0·0056	0·0016
C_2	0·0295	0·0476	0·0451	0·0030	0·0003	0·0009
C_3	0·0361	0·0531	0·0503	0·0069	−0·0028	0·0032
C_4	0·0430	0·0424	0·0424	0·0022	0·0028	0·0057
C_5	0·0405	0·0415	0·0399	−0·0029	0·0028	0·0018
C_6	0·0321	0·0431	0·0408	−0·0023	0·0022	0·0001
C_7	0·0275	0·0385	0·0381	−0·0008	0·0053	0·0015
C_8	0·0376	0·0394	0·0389	−0·0017	0·0043	0·0027
C_9	0·0410	0·0456	0·0450	0·0044	0·0012	0·0052
C_{10}	0·0544	0·0499	0·0496	0·0076	−0·0015	0·0090
C_{11}	0·0666	0·0430	0·0436	0·0006	0·0013	0·0095
C_{12}	0·0619	0·0470	0·0436	−0·0059	−0·0016	0·0026
C_{13}	0·0464	0·0481	0·0438	−0·0049	−0·0016	−0·0004
N	0·0301	0·0397	0·0387	−0·0016	0·0044	0·0010
O	0·0290	0·0659	0·0575	0·0059	−0·0102	−0·0039
Cl	0·0547	0·0586	0·0500	−0·0064	−0·0082	−0·0040

vibrations is not unreasonable. However, two points must be stressed: since the molecule is nearly planar and the nitrogen atom likely to be strongly conjugated to its phenyl group we may assume *a priori* that the two benzene rings librate in phase rather than independently. However, while the major librating axis has been found to lie along the length of the molecule a decision between in-phase and independent vibrations cannot be based on the rigid-body analysis just presented. Secondly, since the anomalous-dispersion correction of the chlorine scattering function was not applied in the least-squares analysis the temperature factor of chlorine must be regarded with reserve.

Small oscillations of r.m.s. amplitude θ about an axis cause the calculated position of an atom, whose distance from this axis is r, to be displaced towards the libration axis by approximately $\frac{1}{2}r\theta^2$. The maximum changes in bond lengths have been found to be 0·001 and 0·006 Å for the low- and room-temperature data, respectively. The libration-corrected bond lengths of the room-temperature structure are listed in Table 11.

TABLE 11.

Bond lengths (room temperature) corrected for thermal vibration.		Standard deviation of bond lengths (Å).	
Bond	Length (Å)	Low temp.	Room temp.
C_1–C_2	1·423	0·0069	0·0059
C_2–C_3	1·399	0·0071	0·0062
C_3–C_4	1·366	0·0071	0·0064
C_4–C_5	1·411	0·0074	0·0063
C_5–C_6	1·361	0·0073	0·0059
C_6–C_1	1·411	0·0069	0·0057
C_1–C_7	1·445	0·0070	0·0058
C_7–N	1·273	0·0066	0·0053
N–C_8	1·420	0·0068	0·0053
C_8–C_9	1·415	0·0076	0·0062
C_9–C_{10}	1·368	0·0073	0·0069
C_{10}–C_{11}	1·390	0·0074	0·0072
C_{11}–C_{12}	1·377	0·0076	0·0074
C_{12}–C_{13}	1·405	0·0074	0·0071
C_8–C_{13}	1·391	0·0075	0·0063
C_5–Cl	1·759	0·0056	0·0046
C_2–O	1·356	0·0060	0·0054

The results of this analysis (molecular shape, packing arrangement, bond lengths, and angles) are discussed in Part X (following paper) where they are compared with the data on 2-chloro-*N*-salicylideneaniline.

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