composition clearly calls for more than one oxidation state. The existence of three different oxidation states is highly unlikely. However, KCr_3O_8 contains both Cr(III) and Cr(VI) (Wilhelmi, 1958), and the bond lengths in $Ba_2Cr_{6\cdot5}O_{14}$ are consistent with Cr(III) in the octahedral sites and Cr(VI) in the tetrahedral sites. With this assumption, charge balance requires that some cation sites be unoccupied, which is consistent with the reduced occupancy factor found for chromium in the tetrahedral sites.

The sum of electrostatic bond strengths assuming the above oxidation states and occupancy is given in Table 2. The value of $2\frac{5}{8}$ to O(3) is, of course, quite high. It should be noted, however, that where a chromium atom has bonds to O(3), these bonds are appreciably longer than its bonds to O(2) or O(1): Cr(1)–O(2)= 1·93 *vs.* Cr(1)–O(3)=1·97; Cr(3)–O(1)=1·64 *vs.* Cr(3)–O(3)=1·71. The bond lengthening would, in effect, decrease the high sum of electrostatic bond strengths.

Atomic parameters are listed for initial and final positions in Table 1. The maximum shift to error ratio in the final cycle was 0·035. Table 3 lists some interatomic distances and bond angles, and Table 4 lists observed and calculated structure factors.

A stereoscopic view of the barium coordination is shown in Fig. 2. The coordination of the three types of chromium, [Cr(1) is ^{VI}Cr(III), Cr(2) is ^{VI}Cr(III), and Cr(3) is ^{IV}Cr(VI)], is shown in Fig. 3.

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The Crystal Structure of 3-Phenyl-2,4-(1*H*,3*H*)-quinazolinedione

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The crystal structure of 3-phenyl-2,4-(1*H*,3*H*)-quinazolinedione, $C_{14}H_{10}N_2O_2$, has been determined from three-dimensional photographic data. The crystals are monoclinic and the space group is $P2_1/c$ with four molecules in the unit cell. The axial parameters are $a=5\cdot799\pm0\cdot002$, $b=8\cdot339\pm0\cdot009$, $c=22\cdot962\pm0\cdot007$ Å, and $\beta=94\cdot16\pm0\cdot04°$. The structure was deduced from a sharpened Patterson synthesis and refined by means of the block-diagonal least-squares method to the final R index of 0·104 for 2255 independent non-zero reflexions. The molecules are placed in pairs around a centre of symmetry, connected by two C=O···H–N hydrogen bonds of length 2·821 Å. The quinazoline rings are superimposed at the intervals of 3·5 Å along the b axis, with their long axes approximately parallel to the [001] direction. The benzene ring is rotated by 65·0° from the quinazoline ring because of the steric effect of the two carbonyl groups.

Introduction

3-Phenyl-2,4(1*H*,3*H*)-quinazolinedione is a model compound of polyquinazolinedione, one of the polymers having the properties of thermal stability and solubility in polyphosphoric acid and organic polar solvents, which were prepared by the cyclopolycondensation reaction of the open-chain precursor (Tohyama, Kurihara, Ikeda & Yoda, 1967; Yoda, 1968, 1969). It was prepared by the reaction of anthranilic acid and phenyl isocyanate in the presence of polyphosphoric acid (PPA) (Kurihara & Yoda, 1965, 1966).

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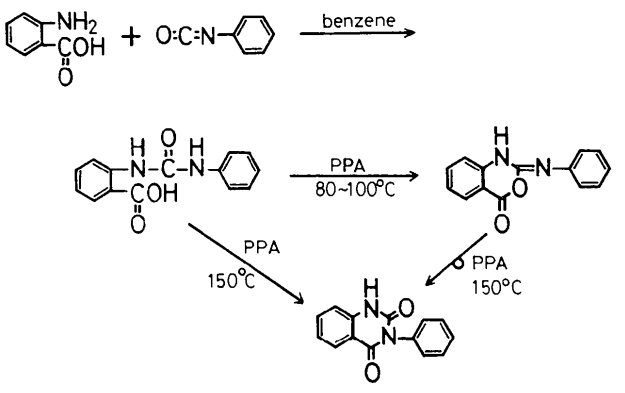

It crystallizes in two modifications, namely a stable form from ethanol solution, and an unstable form from methanol solution, the latter being monoclinic with cell parameters:

$a=7{\cdot}45\pm0{\cdot}05$, $b=8{\cdot}81\pm0{\cdot}02$, $c=15{\cdot}26\pm0{\cdot}05$ Å, $\beta=103{\cdot}1\pm0{\cdot}5°$.

The present paper describes the refinement and crystal structure of the stable form of the molecule.

Experimental

Single crystals of 3-phenyl-2,4-(1*H*,3*H*)-quinazolinedione were grown by slow evaporation at room temperature of an ethanol solution. They were plates tabular on (100) elongated in the **b** direction. The cell dimensions were obtained by a least-squares procedure from the measurements on Weissenberg photographs around the *a* and the *b* axes. The density was measured by flotation in an aqueous solution of sodium acetate at 25 °C.

Crystal data

3-Phenyl-2,4(1*H*,3*H*)-quinazolinedione, $C_{14}H_{10}N_2O_2$
Molecular weight, 238·1, m.p. 280 °C.

Monoclinic
$a = 5{\cdot}799\pm0{\cdot}002$ Å
$b = 8{\cdot}339\pm0{\cdot}009$
$c = 22{\cdot}962\pm0{\cdot}007$
$\beta = 94{\cdot}16\pm0{\cdot}04°$
$V = 1154{\cdot}36$ Å^3
$D_m = 1{\cdot}369$, $D_x = 1{\cdot}370$ g.cm^{-3} for $Z=4$
Systematic absences, $h0l$ with $l=2n+1$
$0k0$ with $k=2n+1$
Space group $P2_1/c$ (No. 14, C_{2h}^5)
Absorption coefficient for Cu $K\alpha$: $\mu=7{\cdot}9$ cm^{-1}.

Three-dimensional intensity data were collected from the equi-inclination Weissenberg photographs taken with Ni-filtered Cu $K\alpha$ radiation. The multiple-film technique was used and zero to the fifth layers about both the *a* and *b* axes were recorded. The intensities were estimated visually by comparison with a calibrated intensity scale prepared from the same crystal. The usual Lorentz and polarization factors were applied to 2255 independent intensities to yield relative structure factors. The crystals used for the intensity measurements were cut to dimensions $0{\cdot}35\times0{\cdot}15\times0{\cdot}15$ mm for the *a* axis, and $0{\cdot}12\times0{\cdot}27\times0{\cdot}15$ mm for the *b* axis, and no corrections were made for the small absorption errors.

Structure determination and refinement

The length of the *c* axis and the sharpened Patterson projection $P(U0W)$ made it almost certain that the molecule was nearly fully extended, with its long axis elongated in the **c** direction. As a first approximation in interpreting the structure, it was assumed that the molecule was almost coplanar. Two pairs of hexagonal patterns of the peaks near the origin of the Patterson projection shown in Fig. 1 indicated that the plane of the molecule would be tilted to some extent from the (010) plane and the long axis tilted about 10° from the [001] direction. Among several models tried, one, also shown in Fig. 1, was adopted by considering the relative heights of the peaks.

With the orientation of the nucleus fixed, an attempt

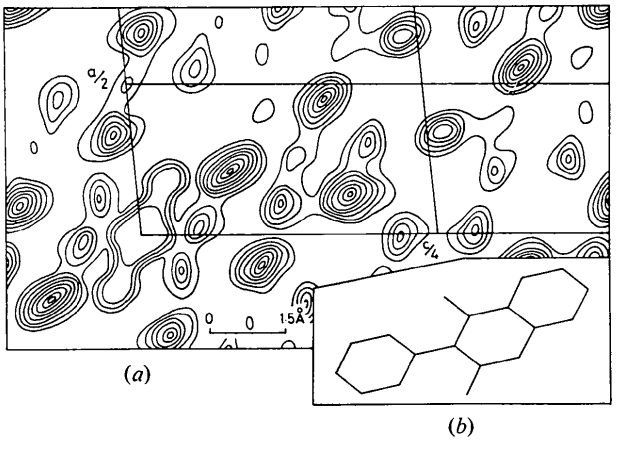

Fig. 1. (*a*) Sharpened Patterson projection $P(U0W)$, with origin peak removed. Contours are drawn at arbitrary intervals. (*b*) Interpretation of (*a*): relative orientation of molecule. The scale is one half of (*a*).

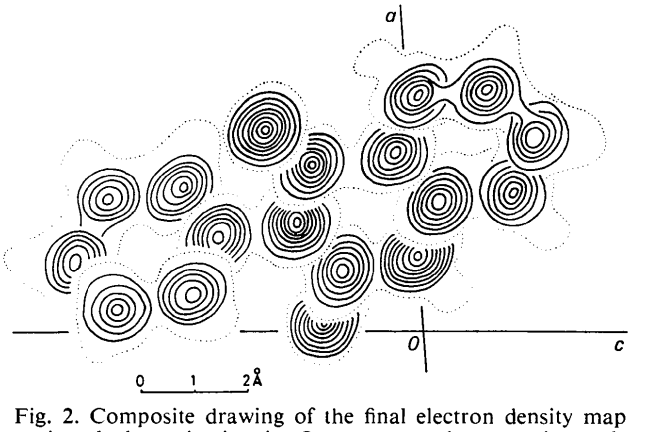

Fig. 2. Composite drawing of the final electron density map viewed along the *b* axis. Contours are drawn at intervals of 1 e.Å^{-3}. The zero line is dotted.

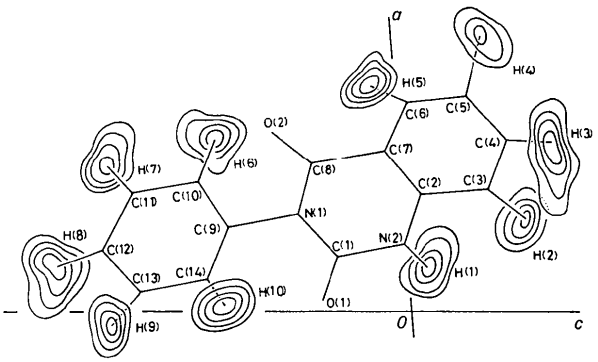

Fig. 3. Electron density peaks associated with the hydrogen positions. Contours are drawn at intervals of 0·2 e.Å^{-3}, starting at 0·2 e.Å^{-3}.

was made to locate the molecules relative to the origin. The molecules were assumed to be joined together in pairs by hydrogen bonds around the centre of symmetry. Several kinds of packing were considered with the aid of molecular models and successive structure factor and Fourier calculations based on 119 $h0l$ reflexions provided an approximate solution of the structure. A further least-squares refinement with a uniform isotropic temperature factor $B=3{\cdot}5$ Å^2 reduced the R index to 0·301 from 0·381.

After obtaining approximate values for the x and z coordinates, the sharpened Patterson projection down the a axis was calculated to determine the y parameters. As a result, no further practical information about the location of the molecule was obtained from the $P(0VW)$ map in which most of the vectors overlapped to a great extent. Attention was then turned to the three-dimensional sharpened Patterson synthesis. The concentration of the vector peaks in the plane through the origin, which is approximately parallel to the $(1\bar{2}1)$ plane suggested the orientation of the molecules in sheets. The strong $1\bar{2}1$ reflexion further supported the orientation. To interpret the distribution of the vector peaks, two possible models which are different in the z coordinates were constructed on the basis of the assumption that the two molecules related by a centre of symmetry are hydrogen bonded, and with the aid of the two-dimensional refinement. The structure factor calculation using the 809 reflexions having $\sin\theta/\lambda \leq 0{\cdot}5$ resulted in an R index of about 0·60 for one model and 0·52 for the other. A further least-squares refinement of the positional parameters yielded no significant improvements in either models. Accordingly a further assumption was made on the latter model that the benzene ring coordinated to the nitrogen atom did not lie on the same plane of the quinazoline ring because of the steric effect of the two carbonyl groups. By the rotation of the benzene ring by about 90° to the quinazoline ring plane the R index decreased to 0·44. Four cycles of least-squares refinement made the angle decrease successively and the R index reduced from 0·33 to 0·27, 0·22 and 0·16. The peaks on the Fourier synthesis calculated at this stage were well resolved and thus this model was considered to be reasonable. The next least-squares computations were based on the complete set of three-dimensional data and three cycles of refinement using individual isotropic temperature factors and allowing variation of all positional parameters reduced the R index from 0·230 to 0·202. Inspection of the calculated curvatures of the atomic peaks showed some anisotropy. After four cycles of positional and anisotropic ther-

Table 1. *The atomic coordinates of* 3-*phenyl*-2,4(1*H*,3*H*) *quinazolinedione*

Standard deviations are in parentheses.

	x/a	y/b	z/c
C(1)	0·1976 (4)	0·0985 (4)	−0·0605 (4)
C(2)	0·4221 (5)	0·2208 (4)	0·0216 (4)
C(3)	0·4469 (5)	0·2475 (5)	0·0820 (5)
C(4)	0·6341 (6)	0·3339 (6)	0·1053 (6)
C(5)	0·7993 (6)	0·3962 (5)	0·0689 (6)
C(6)	0·7699 (5)	0·3718 (6)	0·0091 (5)
C(7)	0·5811 (4)	0·2849 (4)	−0·0146 (4)
C(8)	0·5438 (4)	0·2634 (4)	−0·0785 (4)
C(9)	0·3087 (4)	0·1429 (5)	−0·1596 (4)
C(10)	0·4688 (6)	0·0560 (6)	−0·1880 (5)
C(11)	0·4186 (5)	0·0288 (8)	−0·2488 (6)
C(12)	0·2230 (6)	0·0929 (7)	−0·2781 (7)
C(13)	0·0715 (6)	0·1847 (5)	−0·2482 (6)
C(14)	0·1132 (5)	0·2114 (6)	−0·1882 (5)
N(1)	0·3538 (4)	0·1697 (4)	−0·0972 (5)
N(2)	0·2388 (4)	0·1310 (4)	−0·0021 (4)
O(1)	0·0397 (5)	0·0149 (4)	−0·0786 (4)
O(2)	0·6655 (4)	0·3236 (4)	−0·1133 (4)
H(1)	0·179	0·055	0·021
H(2)	0·338	0·236	0·112
H(3)	0·629	0·351	0·144
H(4)	1·001	0·394	0·083
H(5)	0·853	0·429	−0·018
H(6)	0·611	0·016	−0·165
H(7)	0·557	−0·045	−0·266
H(8)	0·200	0·060	−0·317
H(9)	−0·042	0·268	−0·269
H(10)	0·024	0·297	−0·168

Table 2. *Thermal parameters* (Å^2) *for the expression* $\exp[-(B_{11}h^2+B_{22}k^2+B_{33}l^2+B_{12}hk+B_{13}hl+B_{23}kl)]$.

All values are multiplied by 10^4. Standard deviations are given in parentheses. An isotropic temperature factor $B=2{\cdot}5$ (Å^2) was assigned to all hydrogen atoms.

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
C(1)	204 (8)	91 (4)	9 (2)	−8 (8)	52 (4)	15 (2)
C(2)	196 (5)	83 (4)	8 (2)	45 (8)	47 (4)	18 (2)
C(3)	262 (8)	122 (4)	10 (2)	56 (7)	33 (3)	13 (2)
C(4)	318 (8)	162 (4)	11 (2)	57 (8)	27 (4)	12 (5)
C(5)	312 (7)	184 (5)	12 (2)	−42 (9)	16 (5)	4 (5)
C(6)	232 (6)	145 (5)	12 (2)	−47 (6)	25 (4)	−3 (2)
C(7)	193 (5)	85 (5)	10 (2)	17 (6)	38 (4)	5 (2)
C(8)	163 (5)	94 (4)	8 (2)	−6 (7)	48 (5)	11 (2)
C(9)	222 (7)	90 (5)	8 (2)	−53 (7)	56 (4)	5 (2)
C(10)	336 (7)	117 (5)	12 (2)	87 (8)	78 (4)	9 (2)
C(11)	490 (9)	151 (4)	12 (2)	53 (9)	105 (3)	−4 (4)
C(12)	376 (6)	181 (4)	12 (2)	−140 (9)	36 (4)	−20 (4)
C(13)	277 (6)	238 (4)	13 (2)	−97 (9)	−8 (4)	−19 (5)
C(14)	205 (5)	159 (5)	13 (2)	−44 (6)	26 (4)	−3 (5)
N(1)	187 (5)	94 (5)	7 (2)	−35 (5)	43 (2)	9 (2)
N(2)	216 (5)	108 (4)	8 (2)	−51 (5)	54 (2)	12 (2)
O(1)	270 (5)	140 (5)	10 (2)	−205 (5)	47 (2)	6 (2)
O(2)	213 (5)	140 (4)	10 (2)	−114 (5)	51 (2)	12 (2)

mal parameter refinement the R index decreased to 0·132. A difference Fourier synthesis, using structure factors calculated without hydrogen atoms, clearly showed the presence of the ten hydrogen atoms with the restriction that the peak for H(3) appeared to be anomalously large. The hydrogen atom positions were obtained from the maxima of these peaks. Inclusion of the hydrogen atom contributions to the structure factors reduced the overall agreement index to 0·104 including all non-zero reflexions. Refinement was terminated when nearly all of the parameter shifts were less than the standard deviations. Throughout the refinement of the structure, equal weights were employed for all reflexions and the atomic scattering factors were adopted from *International Tables for X-ray Crystallography* (1962). Composite drawings of the final Fourier and difference maps with atomic levels are shown in Figs. 2 and 3. The fractional coordinates

Table 3. *Observed and calculated structure factors*

The running indices are h, k; the value for l immediately precedes the group. The central column is 10 $|F_o|$, the right-hand column 10 F_c.

H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL
				2	7	48	-48	-1	2	855	897	0	1	120	-126	6	2	16	-20	-4	7	10	5	-5	9	8	4	3	2	104	81
	L = 0			2	8	58	65	-1	3	232	178	0	2	102	90	6	3	32	31	-4	8	9	-2	4	1	65	-51	3	3	53	25
				2	9	30	37	-1	4	120	90	0	3	28	7	6	4	14	-9	-4	9	42	34	4	2	157	127	3	4	13	22
0	2	628	-683	2	10	6	-5	-1	5	53	-62	0	4	144	130	-6	1	71	-57	5	0	66	63	4	3	55	52	3	5	38	-31
0	4	57	-71	-2	1	249	284	-1	6	18	10	0	5	62	-48	-6	2	158	-146	5	1	36	33	4	4	73	-75	3	6	116	-132
0	6	71	74	-2	2	370	329	-1	7	63	59	0	6	237	-212	-6	3	47	-44	5	2	68	66	4	5	14	17	3	7	10	-2
0	8	75	71	-2	3	239	197	-1	8	10	-15	0	7	28	28	-6	4	18	5	5	3	30	35	4	6	71	76	3	8	53	57
0	10	7	-12	-2	4	346	-353	-1	9	54	-14	0	8	58	64	-7	2	88	94	5	4	50	40	4	7	10	2	3	9	44	52
1	0	772	-820	-2	5	69	64	-1	10	7	-16	0	9	8	20					5	5	11	3	4	8	8	1	-3	1	265	281
1	1	317	-339	-2	6	9	1	2	1	99	59	0	10	33	-41		L = 4			5	6	44	48	-4	1	9	8	-3	2	216	-190
1	2	594	597	-2	7	60	56	2	2	288	-254	1	1	57	65					5	7	8	15	-4	2	56	62	-3	3	38	12
1	3	209	-196	-2	8	34	-37	2	3	8	-8	1	2	232	-168	0	0	349	300	-5	1	73	-87	4	3	69	-61	-3	4	53	-38
1	4	192	-167	-2	9	68	-64	2	4	528	521	1	3	52	27	0	1	241	-211	-5	2	284	-196	-4	4	151	-148	-3	5	95	-85
1	5	22	-18	-2	10	6	8	2	5	104	101	1	4	52	81	0	2	204	160	-5	3	86	-85	4	5	103	-86	-3	6	208	-192
1	6	85	79	3	1	186	195	2	6	167	-155	1	5	25	27	0	3	90	70	-5	4	62	48	-4	6	102	82	-3	7	104	89
1	7	29	36	3	2	67	53	2	7	25	-21	1	6	219	211	0	4	12	19	-5	5	36	23	4	7	10	6	-3	8	100	104
1	8	10	23	3	3	104	98	2	8	43	47	1	7	43	35	0	5	30	20	-5	6	62	61	-4	8	84	71	-3	9	8	15
1	9	23	-28	3	4	98	82	2	9	9	-12	1	8	63	63	0	6	176	-169	-5	7	10	11	4	9	6	7	4	0	113	116
1	10	76	82	3	5	169	156	2	10	35	43	1	9	45	-43	0	7	9	14	6	0	30	17	5	1	31	-3	4	1	41	-28
2	0	64	-65	3	6	262	-252	-2	0	584	-493	1	10	7	14	0	8	48	56	6	1	39	20	5	2	59	-66	4	2	137	-99
2	1	267	-270	3	7	30	35	-2	1	223	244	-1	1	308	280	0	9	8	-31	6	2	54	39	5	3	21	27	4	3	13	-15
2	2	86	-70	3	8	108	106	-2	2	54	-52	-1	2	273	-258	0	10	46	52	6	3	28	-35	5	4	137	157	4	4	63	-72
2	3	182	153	3	9	8	16	-2	3	266	-251	-1	3	270	237	1	0	463	425	6	4	56	55	5	5	11	21	4	5	24	19
2	4	699	724	-3	1	66	-77	-2	4	128	123	-1	4	391	-388	1	1	350	-324	-6	0	463	-514	5	6	35	-27	4	6	86	98
2	5	69	51	-3	2	192	145	-2	5	192	-193	-1	5	169	-174	1	2	26	-8	-6	1	74	62	5	7	33	33	4	7	47	49
2	6	75	-62	-3	3	59	33	-2	6	69	59	-1	6	26	-16	1	3	148	144	-6	2	148	125	-5	1	113	-147	-4	0	14	32
2	7	10	-10	-3	4	235	230	-2	7	23	-26	-1	7	32	-28	1	4	503	-492	-6	3	14	7	-5	2	312	-308	-4	1	13	-27
2	8	20	-24	-3	5	124	-115	-2	8	36	-39	-1	8	109	116	1	5	138	123	-6	4	37	14	-5	3	60	56	-4	2	161	161
2	9	65	70	-3	6	212	-207	-2	9	47	-43	-1	9	9	1	1	6	43	45	7	0	10	20	5	4	30	12	-4	3	62	-59
2	10	29	-31	-3	7	63	49	-2	10	44	-43	-1	10	111	-131	1	7	10	-6	7	0	43	40	-5	5	88	-73	-4	4	296	-311
3	0	85	48	-3	8	10	-5	3	0	69	-36	2	1	141	-108	1	8	10	-14	7	2	56	-62	-5	6	108	80	-4	5	52	42
3	1	83	-67	-3	9	8	12	3	1	281	304	2	2	481	-405	1	9	9	52					-5	7	36	29	-4	6	108	102
3	2	62	-39	4	1	71	97	3	2	268	235	2	3	398	392	1	10	7	9		L = 5			6	1	30	59	-4	7	10	-1
3	3	100	94	4	2	77	82	3	3	18	-14	2	4	14	-22	-1	0	31	-15					6	2	60	56	-4	8	8	11
3	4	49	-36	4	3	115	120	3	4	93	79	2	5	11	-20	-1	1	232	-241	0	1	97	78	6	4	35	-17	5	0	57	-70
3	5	117	-103	4	4	150	146	3	5	116	-101	2	6	194	156	-1	2	697	-726	0	2	336	371	6	1	69	53	5	1	38	19
3	6	296	-300	4	5	78	76	3	6	182	177	2	7	84	86	-1	3	371	-340	0	3	343	360	6	2	95	73	5	2	25	-24
3	7	80	-69	4	6	10	8	3	7	123	123	2	8	53	-58	-1	4	39	-15	0	4	220	223	6	3	14	5	5	3	14	1
3	8	59	-64	4	7	88	71	3	8	111	-120	2	9	44	42	-1	5	125	-109	0	5	50	43	6	4	36	26	5	4	14	11
3	9	8	-11	4	8	135	-116	3	9	30	28	2	10	22	26	-1	6	110	104	0	6	52	-43	-7	2	126	137	5	5	11	-17
4	0	14	16	4	9	23	-23	-3	0	47	-20	-2	1	210	-196	-1	7	43	-43	0	7	44	53					5	6	42	43
4	1	40	-34	-4	1	48	42	-3	1	61	-60	-2	2	87	-28	-1	8	10	-21	0	8	9	24		L = 6			5	7	28	27
4	2	192	205	-4	2	77	60	-3	2	68	-56	-2	3	463	430	-1	9	9	-18	0	9	8	-22					-5	1	18	18
4	3	73	56	-4	3	179	161	-3	3	60	-56	-2	4	139	-113	-1	10	100	-100	0	10	28	-37	0	0	634	671	5	2	188	190
4	4	73	-58	-4	4	98	-79	-3	5	156	137	-2	5	80	62	2	0	355	310	1	1	279	-265	0	1	155	-147	5	3	13	-3
4	5	82	69	-4	5	101	89	-3	6	68	-58	-2	6	157	154	2	1	106	-77	1	2	395	361	0	2	152	-139	5	4	112	86
4	6	136	-126	-4	6	43	33	-3	7	30	-25	-2	7	35	37	2	2	120	-84	1	3	17	23	0	3	24	-13	5	5	41	32
4	7	10	-8	-4	7	10	-11	-3	8	10	-16	-2	8	175	-183	2	3	29	-27	1	4	152	-112	0	4	275	-281	5	6	11	-12
4	8	84	76	-4	9	6	-6	-3	9	21	-26	-2	9	38	-38	2	4	198	166	1	5	54	-51	0	5	167	152	-5	7	10	1
4	9	24	-25	5	1	57	48	4	0	230	-220	-2	10	61	63	2	5	19	-21	1	6	94	80	0	6	47	-50	6	0	77	-84
5	0	108	116	5	2	25	-6	4	1	28	-23	3	1	59	71	2	6	28	-23	1	7	63	-62	0	7	9	-11	6	1	38	37
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5	6	57	-50	5	7	10	-36	4	6	30	24	3	6	60	-48	-2	1	73	36	-1	2	196	-171	1	1	16	20	6	3	14	-27
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6	0	79	-63	-5	2	19	-14	4	8	146	139	3	8	98	100	-2	3	85	56	-1	4	36	19	1	3	132	-113	7	0	66	88
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7	0	44	-50	-5	4	107	-105	-4	1	131	121	-3	1	8	15	2	5	115	98	-1	6	9	8	1	5	49	51	-7	2	47	-50
7	2	37	-42	-5	5	14	5	-4	2	104	109	-3	2	212	207	-2	6	164	187	-1	7	22	23	1	6	54	-55				
	L = 1			-5	6	11	-5	-4	3	96	107	-3	3	76	54	-2	7	33	26	-1	8	95	92	1	7	23	22		I = 7		
				-5	7	10	1	-4	4	178	175	-3	4	132	113	-2	8	214	197	-1	9	9	18	1	8	25	31				
				6	1	31	2	-4	5	139	128	-3	5	141	110	-2	9	49	51	-1	10	107	-137	1	9	43	-46	0	1	137	135
0	1	349	338	6	2	79	81	-4	6	10	-5	-3	6	215	-202	-2	10	6	12	2	1	38	56	1	10	20	-30	0	2	34	23
0	2	872	909	6	3	36	38	-4	7	10	-18	3	7	105	-99	3	0	716	-682	2	2	427	-371	-1	0	179	-173	0	3	192	-199
0	3	257	230	6	4	14	5	-4	8	9	-4	-3	8	10	-12	3	1	33	32	2	3	125	-105	-1	1	279	-291	0	4	124	119
0	4	135	115	-6	1	35	4	-4	9	30	-30	-3	9	33	-39	3	2	290	258	2	4	232	211	-1	2	402	-391	0	5	210	-211
0	5	28	11	6	2	79	82	5	0	134	140	4	1	147	140	3	3	43	33	2	5	88	-76	-1	3	119	123	0	6	116	-112
0	6	43	48	-6	3	14	-12	5	1	75	-80	4	2	206	199	3	4	123	92	2	6	43	25	-1	4	63	73	0	7	9	16
0	7	69	70	-6	4	37	-33	5	2	62	53	4	3	29	14	3	5	74	64	2	7	66	-67	-1	5	206	169	0	8	9	-19
0	8	52	54	-7	2	36	35	5	3	52	48	4	4	102	-98	3	6	56	43	2	8	32	28	-1	6	25	-22	0	9	8	14
0	9	8	9	-7	2	31	20	5	4	37	-36	4	5	76	66	3	7	30	39	2	9	8	-5	1	7	10	4	0	10	5	-7
0	10	6	-1					5	5	65	53	4	6	10	17	3	8	10	6	2	10	51	55	-1	8	10	29	1	1	265	-247
1	1	659	738		L = 2			5	6	11	34	4	7	50	39	3	9	21	-18	-2	1	127	-143	-1	9	27	-40	1	2	248	-188
1	2	1045	-1106					5	7	9	12	4	8	53	-41	-3	0	111	-79	-2	2	115	-75	-1	10	83	-87	1	3	77	-45
1	3	208	-191	0	0	692	776	-5	1	113	137	-4	1	127	-167	-3	1	118	-119	-2	3	146	154	2	0	87	43	1	4	45	-22
1	4	87	67	0	1	525	584	-5	2	227	-254	-4	2	208	234	-3	2	182	-140	-2	5	68	-69	2	1	219	232	1	5	175	-174
1	5	209	236	0	2	448	-502	-5	3	13	-17	-4	3	83	-77	-3	3	37	28	-2	6	10	-7	2	2	213	-129	1	6	127	127
1	6	122	109	0	3	26	39	-5	4	21	-25	-4	4	188	193	-3	4	232	208	-2	7	121	-131	2	3	184	149	1	7	29	-37
1	7	10	9	0	4	97	-66	-5	5	14	-4	-4	5	62	-58	-3	5	71	-67	-2	8	241	-227	2	4	52	-40	1	8	83	-77
1	8	63	-69	0	5	53	-59	-5	6	72	-65	-4	6	30	-35	-3	6	345	-359	-2	9	9	-12	2	5	79	-68	1	9	9	-15
1	9	9	30	0	6	73	-50	-5	7	34	23	-4	7	78	-61	-3	7	150	-150	-2	10	58	63	2	6	100	-104	1	10	6	-9
1	10	7	-14	0	7	134	142	6	0	44	49	-4	8	29	-40	-3	8	41	37	3	1	66	47	2	7	26	30	-1	1	33	-11
-1	1	316	-328	0	8	123	139	6	1	39	49	-4	9	54	50	-3	9	8	-15	3	2	48	-25	2	8	113	116	-1	2	308	-278
-1	2	1025	-1161	0	9	88	5	6	2	35	20	5	1	29	23	4	0	218	218	3	3	125	-120	2	9	8	5	-1	3	222	-194
-1	3	296	295	0	10	19	25	6	3	29	16	5	2	38	-38	4	1	17	-12	3	4	86	80	2	10	54	71	-1	4	241	220
-1	4	478	488	1	0	185	165	6	4	14	33	5	3	43	61	4	2	82	-79	3	5	48	41	-2	0	714	-732	-1	5	24	25
-1	5	79	73	1	1	255	199	-6	0	154	-164	5	4	83	84	4	3	48	37	3	6	111	-28	-2	1	210	-162	-1	6	39	32
-1	6	58	56	1	2	1068	1103	-6	1	127	-108	5	5	11	-1	4	4	74	55	3	7	86	89	-2	2	255	214	-1	7	10	-21
-1	7	10	5	1	3	36	-18	6	2	83	83	5	6	10	20	4	5	76	73	3	8	99	117	-2	3	81	-17	-1	8	10	3
-1	8	100	98	1	4	369	347	-6	3	14	-19	5	7	9	11	4	6	57	58	3	9	8	9	-2	4	104	-96	-1	9	83	-83
-1	9	21	51	1	5	131	122	-6	4	43	-43	-5	1	83	93	4	7	33	-35	-3	1	217	-220	-2	5	106	-84	1	10	66	-81
-1	10	54	-58	1	6	161	134	7	0	10	-3	-5	2	231	-267	4	8	8	23	-3	2	208	202	-2	6	80	-72	2	1	232	-228
2	1	95	63	1	7	10	-1	7	2	25	23	5	3	140	-151	-4	1	71	-89	-3	3	134	-141	-2	7	68	-68	2	2	79	-45
2	2	153	153	1	8	27	30	-7	0	11	14	-5	4	103	99	4	2	35	26	-3	4	27	30	2	8	201	-178	2	3	121	-126
2	3	162	151	1	9	37	6	-7	2	106	-140	-5	5	34	-27	-4	3	118	124	-3	5	180	-155	-2	9	8	11	2	4	81	79
2	4	283	-323	1	10	7	16					-6	6	31	21	-4	4	438	-483	-3	6	333	-322	-2	10	44	47	2	5	110	100
2	5	96	82	-1	0	879	-892		L = 3			-5	7	10	-12	-4	5	49	-33	-3	7	26	-28	3	0	229	-213	2	6	20	27
2	6	290	272	-1	1	362	402					6	1	13	19	-4	6	82	64	-3	8	95	95	3	1	61	-55	2	7	84	-90

Table 3 (*cont.*)

H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL
2	8	38	-45	-1	9	9	-18	1	4	139	146	1	0	808	779						0	1	188	156	-6	1	54	-48	0	3	37	-22
2	9	8	8	-1	10	14	-42	1	5	31	-33	1	1	48	76		L = 11				0	2	76	-53	-6	2	80	74	0	4	[illegible]	-57
-2	1	453	-417	2	0	222	-176	1	6	10	-3	1	2	320	260						0	3	30	15	-6	3	65	55	0	5	107	-104
-2	2	342	302	2	1	186	-183	1	7	25	23	1	3	89	58	0	1	318	297	0	4	100	86	-6	4	40	36	0	6	158	-176
-2	3	33	24	2	2	125	-111	1	8	118	-107	1	4	126	101	0	2	366	-297	0	5	12	27					0	7	49	55
-2	4	200	168	2	3	152	-115	1	9	8	-37	1	5	61	40	0	3	13	16	0	6	43	43		L = 13			0	8	153	159
-2	5	104	-88	2	5	76	60	1	10	19	-31	1	6	10	7	0	4	42	50	0	7	59	71					0	9	32	46
-2	6	28	27	2	6	10	-8	-1	1	73	29	1	7	51	13	0	5	54	43	0	8	85	117	0	1	108	130	1	0	214	206
-2	7	48	-34	2	7	21	-17	-1	2	292	-261	1	8	91	89	0	6	84	-84	0	9	39	-53	0	2	123	111	1	1	58	-75
-2	8	71	-63	2	8	104	-99	-1	3	166	-142	1	9	8	4	0	7	9	13	1	0	114	-71	0	3	70	-73	1	2	265	250
-2	9	8	8	2	9	8	-18	-1	4	463	467	1	10	53	37	0	8	7	23	1	1	163	-152	0	4	107	-99	1	3	45	-38
-2	10	66	66	2	10	49	73	-1	5	71	58	-1	0	219	174	0	9	34	-37	1	2	186	167	0	5	104	87	1	4	178	-173
3	1	140	126	-2	0	391	-408	-1	6	88	-55	-1	1	145	126	0	10	21	-35	1	3	124	-99	0	6	9	-2	1	5	136	134
3	2	75	66	-2	1	79	-52	-1	7	10	-13	-1	2	326	276	1	1	79	-42	1	4	73	-74	0	7	157	188	1	6	235	250
3	3	27	-18	-2	2	153	124	-1	8	52	-58	-1	3	23	27	1	2	423	-382	1	5	197	100	0	8	131	171	1	7	29	29
3	4	13	-11	-2	3	184	143	-1	9	8	-21	-1	4	38	14	1	3	25	-17	1	6	118	151	0	9	31	-45	1	8	8	-14
3	5	104	-93	-2	4	28	25	-1	10	31	41	-1	5	30	30	1	4	41	35	1	7	138	-137	1	1	151	124	1	9	6	15
3	6	86	-99	-2	5	161	149	2	1	9	-7	-1	6	10	9	1	5	126	117	1	8	52	-51	1	2	190	-146	-1	0	203	204
3	7	37	-42	-2	6	82	-61	2	2	226	232	-1	7	44	50	1	6	44	35	1	9	22	-24	1	3	149	154	-1	1	10	17
3	8	54	55	-2	7	60	-76	2	3	213	-194	-1	8	10	25	1	7	45	-56	-1	0	12	-47	1	4	272	-272	-1	2	322	290
3	9	7	-10	-2	8	19	21	2	4	222	-201	-1	10	37	55	1	8	46	-46	-1	1	236	-211	1	5	142	142	-1	3	98	-97
-3	1	9	-1	-2	9	43	43	2	5	55	-80	2	0	126	95	1	9	30	43	-1	2	227	208	1	6	179	195	-1	4	77	64
-3	2	281	263	-2	10	34	35	2	6	27	29	2	1	106	97	-1	1	78	116	-1	3	167	149	1	7	10	2	-1	5	14	7
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-3	4	46	37	3	1	14	-18	2	8	41	-45	2	3	86	63	-1	3	76	98	-1	5	121	119	1	9	6	-16	-1	7	10	-13
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-3	6	41	-36	3	3	31	-25	-2	1	155	173	2	5	80	75	-1	5	85	81	-1	7	22	-20	-1	2	57	-40	-1	9	6	-6
-3	7	51	53	3	4	13	10	-2	2	387	353	2	6	44	-30	-1	6	10	-11	-1	8	9	-18	-1	3	292	273	2	0	191	-170
-3	8	66	66	3	5	14	3	-2	3	18	15	2	7	53	-62	-1	7	54	59	-1	9	65	-48	-1	4	77	66	2	1	118	106
-3	9	8	-2	3	6	106	-104	-2	4	141	-117	2	8	60	-59	-1	8	9	14	2	0	164	155	-1	5	85	-74	2	2	89	-83
4	1	25	-26	3	7	35	-45	-2	5	12	18	2	9	28	-32	-1	9	45	89	2	1	52	52	-1	6	63	73	2	3	13	2
4	2	65	47	3	8	9	-26	-2	6	104	107	-2	0	55	38	2	1	32	27	2	2	204	-180	-1	7	72	-64	2	4	334	341
4	3	57	41	3	9	26	31	-2	7	25	21	-2	1	80	80	2	2	173	127	2	3	208	179	-1	8	84	81	2	5	77	-76
4	4	75	-71	-3	0	686	676	-2	8	9	-3	-2	2	238	177	2	3	168	159	2	4	314	345	2	1	52	-53	2	6	32	-23
4	5	44	-43	-3	1	150	149	-2	9	7	3	-2	3	35	22	2	4	61	-40	2	5	71	-55	2	2	54	-44	2	7	49	8
4	6	36	31	-3	2	178	-146	3	1	93	-81	-2	4	191	186	2	5	36	-33	2	6	60	-63	2	3	140	138	2	9	4	-37
4	7	9	5	-3	3	22	25	3	2	62	-46	-2	5	119	108	2	6	33	-33	2	7	10	10	2	4	94	96	-2	0	98	-114
-4	1	86	79	-3	4	99	-86	3	3	50	41	-2	6	176	-180	2	7	10	5	2	8	8	-10	2	5	14	6	-2	1	107	95
-4	2	170	-148	-3	5	13	3	3	4	77	64	-2	7	27	33	2	8	9	5	2	9	21	-21	2	6	68	66	2	2	104	-100
-4	3	200	-193	-3	6	27	27	3	5	99	-93	-2	8	65	59	2	9	6	12	-2	0	178	140	2	7	9	-5	-2	3	121	-103
-4	4	55	40	-3	7	57	49	3	6	58	-57	-2	9	8	-14	-2	1	122	87	-2	1	175	170	2	8	59	-61	-2	4	37	36
-4	5	71	63	-3	8	45	-57	3	7	25	-30	3	0	44	30	-2	2	66	49	-2	2	207	170	2	9	22	28	-2	5	132	-118
-4	6	67	48	-3	9	7	-26	3	8	9	-13	3	1	88	95	-2	3	131	100	-2	3	31	21	-2	1	143	142	-2	6	136	151
-4	7	30	-30	4	0	102	-88	3	9	6	-6	3	2	24	-15	-2	4	95	-73	-2	4	229	212	-2	2	157	-158	-2	7	48	42
-4	8	8	10	4	1	55	45	-3	1	25	11	3	3	39	-27	-2	5	70	66	-2	5	70	-62	-2	3	205	195	-2	9	5	1
5	1	33	-20	4	2	65	-58	-3	2	123	-76	3	4	135	-126	-2	6	90	96	-2	6	36	-17	-2	4	157	-143	3	0	287	-318
5	2	92	-120	4	3	13	-2	-3	3	139	137	3	5	14	-7	-2	7	10	-4	-2	7	46	44	-2	5	55	-44	3	1	203	207
5	3	14	-11	4	4	79	-94	-3	4	65	-44	3	6	11	-9	-2	8	38	39	-2	8	16	-21	-2	6	10	21	3	2	274	287
5	4	71	69	4	5	30	-38	-3	5	31	-35	3	7	10	5	-2	9	40	-44	-2	9	6	14	-2	7	45	42	3	3	44	47
5	5	11	-3	4	6	10	2	-3	6	11	-16	3	8	9	-28	3	1	45	-46	3	0	20	-8	-2	8	50	-50	3	4	14	12
5	6	9	-24	4	7	9	18	-3	7	79	-78	3	9	21	-31	3	2	13	2	3	1	36	-14	-2	9	6	1	3	5	14	14
5	7	6	-3	-4	0	98	-71	-3	8	86	79	-3	0	199	171	3	3	27	-40	3	2	119	102	3	1	247	269	3	6	31	36
-5	1	20	-25	-4	1	47	-18	-3	9	44	51	-3	1	61	-65	3	4	120	124	3	3	84	-82	3	2	248	249	3	7	9	4
-5	2	13	-4	-4	2	36	21	4	1	39	-37	-3	2	29	-14	3	5	41	-37	3	4	71	-54	3	3	132	-118	3	8	29	-28
-5	3	54	47	-4	3	51	-48	4	2	31	-18	-3	3	69	55	3	6	149	-158	3	5	52	-51	3	4	53	-47	-3	0	87	-58
-5	4	36	-32	-4	4	25	-21	4	3	128	-136	-3	4	17	34	3	7	10	32	3	6	69	65	3	5	64	64	-3	1	52	48
-5	5	14	1	-4	5	46	36	4	4	126	-143	-3	5	22	-35	-3	1	143	139	3	7	9	19	3	6	94	85	-3	2	45	-54
5	6	160	138	-4	6	10	-28	4	5	24	18	-3	6	160	167	-3	2	147	121	3	8	26	-29	3	7	9	-11	-3	3	97	-102
-5	7	27	-18	-4	7	35	22	4	6	10	11	-3	7	36	48	-3	3	82	61	-3	0	46	-7	3	8	26	26	-3	4	208	231
6	1	32	-40	-4	8	102	86	4	7	8	-18	-3	8	36	-63	-3	4	23	-1	-3	1	26	-54	-3	1	117	100	-3	5	58	63
6	2	60	47	5	0	60	77	-4	1	46	42	-3	9	51	64	-3	5	140	132	-3	2	157	130	-3	2	13	11	-3	6	101	-97
-6	1	39	20	5	1	66	-70	-4	2	187	-149	4	0	72	-70	-3	6	87	-89	-3	3	12	12	-3	3	100	-110	-3	7	9	4
-6	2	31	-36	5	2	93	-103	4	3	39	29	4	1	37	29	-3	7	25	25	-3	4	21	27	-3	4	14	29	-3	8	7	15
-6	3	14	-14	5	3	14	14	-4	4	147	144	4	2	113	125	-3	8	67	78	-3	5	31	27	-3	5	75	57	4	0	400	439
-6	4	68	55	5	4	14	19	-4	5	87	76	4	3	59	-63	-3	9	37	46	-3	6	58	56	-3	6	45	-48	4	1	19	-24
-7	2	46	51	5	5	45	47	-4	6	10	-2	4	4	93	-91	4	1	20	3	-3	7	37	-44	-3	7	10	8	4	2	136	-122
	L = 8			5	6	9	-9	-4	7	86	70	4	5	76	-64	4	2	47	35	-3	8	24	31	-3	8	34	44	4	3	57	-46
				5	7	15	-18	-4	8	77	70	4	6	113	-103	4	3	53	35	-4	0	128	124	4	1	33	32	4	4	14	-17
				-5	0	17	5	5	1	33	-35	4	7	8	14	4	4	14	-11	4	1	163	-185	4	2	14	6	4	5	13	-7
0	0	241	168	-5	1	106	-116	5	2	36	-31	-4	0	53	43	4	5	29	-29	4	2	61	-57	4	3	59	-62	4	6	8	15
0	1	32	-21	-5	2	18	22	5	3	65	-76	-4	1	109	103	4	6	9	10	4	3	48	43	4	4	21	-35	-4	0	44	-49
0	2	327	-284	-5	3	60	52	5	4	14	-8	-4	2	118	96	4	7	33	-35	4	4	14	-9	4	5	39	30	-4	1	57	-56
0	3	133	150	-5	4	109	96	5	5	10	26	-4	3	76	79	-4	1	115	109	4	5	84	67	4	6	8	18	-4	2	57	58
0	4	241	215	-5	5	68	39	5	6	8	28	-4	4	79	75	-4	2	22	8	4	6	42	-55	-4	1	71	-71	-4	3	72	70
0	5	26	-17	-5	6	76	52	-5	1	52	52	-4	5	22	-27	-4	3	108	95	-4	0	119	103	-4	2	111	112	-4	4	122	-124
0	6	252	241	-5	7	9	18	-5	2	78	80	-4	6	34	26	-4	4	14	26	-4	1	94	-95	-4	3	147	154	-4	5	83	-72
0	7	91	108	6	0	135	-147	-5	3	53	37	-4	7	34	43	-4	5	96	-84	-4	2	31	59	-4	4	116	121	-4	6	122	86
0	8	9	-34	6	2	43	47	-5	4	71	-70	-4	8	132	121	-4	6	10	16	-4	3	70	-62	-4	5	63	44	-4	7	8	-45
0	9	8	1	-6	0	15	19	-5	5	59	49	5	0	59	53	-4	7	90	81	-4	4	39	-48	-4	6	30	21	5	0	12	18
0	10	5	5	-6	1	13	13	-5	6	87	70	5	1	20	27	-4	8	7	13	-4	5	22	19	-4	7	9	11	5	1	28	26
1	0	239	181	-6	2	76	-72	-5	7	45	40	5	2	105	-125	5	1	49	-54	-4	6	84	68	-4	8	6	-18	5	2	68	77
1	1	263	207	-6	4	81	75	6	2	61	61	5	3	52	-56	5	2	37	-31	-4	7	9	21	5	1	11	-18	5	3	52	-55
1	2	76	-36	-7	0	55	-75	-6	1	13	23	5	4	46	-49	5	3	46	-51	-4	8	76	53	5	2	122	-130	5	4	67	-67
1	3	121	116	-7	2	110	116	-6	2	15	3	5	5	10	1	5	4	90	-92	5	0	24	-1	5	3	56	54	5	5	22	34
1	4	190	176					-6	4	110	125	5	6	32	31	5	5	59	-68	5	1	11	-15	5	4	77	76	-5	0	243	297
1	5	38	-36		L = 9			-7	2	53	58	-5	0	41	-18	5	6	26	-32	5	2	57	54	5	5	24	29	-5	1	68	88
1	6	169	165									-5	1	12	-10	-5	1	54	50	5	3	12	8	-5	1	14	-8	-5	2	152	-155
1	7	10	11	0	1	403	-363		L = 10			-5	2	80	80	-5	2	46	-44	5	4	24	-13	-5	2	37	-22	-5	3	15	12
1	8	57	56	0	2	248	-208					-5	3	21	-25	-5	3	14	-17	5	5	27	-33	-5	3	13	-1	-5	4	13	-20
1	9	53	58	0	3	181	183	0	0	621	602	-5	4	14	-13	-5	5	87	88	5	6	12	-30	-5	5	11	11	-5	5	25	-25
1	10	71	80	0	4	23	43	0	1	249	196	-5	5	14	25	-5	7	59	44	-5	0	74	67	-5	6	18	18	-5	6	158	-166
-1	0	441	-411	0	5	22	-20	0	2	372	355	-5	6	93	81	6	2	35	-39	-5	1	83	114	-6	1	57	57	-6	1	69	-84
-1	1	121	122	0	6	145	-141	0	3	128	145	-5	7	45	35	-6	1	36	25	-5	2	47	-42	-6	2	52	-53	6	2	92	91
-1	2	137	145	0	7	9	25	0	4	36	32	6	0	56	-63	-6	2	14	9	-5	3	43	-43	-6	4	28	18	6	4	25	-34
1	3	57	44	0	8	41	57	0	5	98	95	6	2	32	-10	-6	3	55	43	-5	4	105	87								
-1	4	124	86	0	9	7	-1	0	6	88	80	-6	0	46	60	-6	4	61	51	-5	5	13	21		L = 14				L = 15		
-1	5	11	16	0	10	5	8	0	7	9	15	-6	1	13	-9					-5	6	11	53								
-1	6	69	53	1	1	54	33	0	8	19	23	-6	2	14	24		L = 12			-5	7	8	12	0	0	55	55	0	1	105	84
-1	7	10	29	1	2	72	-26	0	9	21	26	-6	3	38	39					-6	0	59	-67	0	2	145	144	0	3	90	83
-1	8	41	52	1	3	103	-105	0	10	5	25	-6	4	81	74	0	0	817	800	-6	0	59	-67	0	2	145	144	0	3	90	83

and anisotropic thermal parameters, along with their standard deviations are listed in Tables 1 and 2 respectively, and the final observed and calculated structure factors are given in Table 3.

Results and discussion

Dimensions of the molecule

The intramolecular bond lengths and valence bond angles of the molecule are listed in Table 4 and shown in Fig. 4. The benzene ring has mean a carbon bond distance of 1·396 Å and a mean angle of 120·0°; values range from 1·384 to 1·423 Å and from 116·8 to 123·1°. These values are quite reasonable. The six-membered carbon ring of the quinazoline ring also has a reasonable mean carbon bond distance of 1·394 Å and a mean angle of 120·0°, values ranging from 1·378 to 1·415 Å and from 119·2 to 120·7°. The carbon–carbon bond distance of 1·478 Å in the heterocyclic ring may be compared with 1·475 Å for tricycloquinazoline (Iball & Motherwell, 1969). The mean nitrogen–carbon bond distance of 1·389 Å is similar to those usually observed in heterocyclic rings, for instance, dihydrothymidine (Konnert, Karle & Karle, 1970), dihydrouracil (Rohrer &

Table 3 (*cont.*)

H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL	H	K	KFOB	FCAL
0	4	42	45	1	0	204	168	1	6	144	136	2	8	45	-60	4	2	51	48	-1	5	38	-38	0	2	104	99	1	3	10	6
0	5	41	-29	1	1	65	68	1	7	57	-58	-2	0	858	-939	4	3	34	-37	2	1	76	-81	0	3	48	-46	1	3	29	40
0	6	198	-191	1	2	106	-106	1	8	36	-39	-2	1	194	-215	-4	1	28	-27	2	2	80	-85	0	4	24	-38	-1	1	52	43
0	7	8	-11	1	3	29	23	-1	1	74	65	-2	2	229	208	-4	2	255	-239	2	3	12	20	0	5	38	25	-1	2	34	-31
0	8	85	103	1	4	101	-97	-1	2	353	-354	-2	3	103	-94	-4	4	155	132	2	4	55	43	0	6	5	-14	-1	3	13	7
1	1	14	8	1	6	20	22	-1	3	279	-301	-2	4	32	22	-4	5	13	-1	2	6	6	10	1	1	12	9	-1	4	13	-14
1	2	86	-65	1	7	27	34	-1	4	236	220	-2	5	14	-22	5	2	72	70	-2	1	32	27	1	2	73	57	-1	5	63	59
1	3	39	41	1	8	22	20	-1	5	90	-83	-2	6	25	-14	-5	1	29	30	-2	2	79	74	1	3	66	57	2	1	10	-10
1	4	63	-48	-1	0	121	112	-1	6	10	15	-2	7	47	-50	-5	2	13	-11	-2	3	76	64	1	5	7	-26	2	2	35	-35
1	5	14	11	-1	1	58	61	-1	7	35	42	-2	8	54	-62					-2	4	115	101	1	6	5	-5	2	3	51	49
1	6	134	157	-1	2	366	-365	2	1	12	-7	3	0	52	-38		L = 20			-2	5	65	52	-1	1	36	23	2	4	50	45
1	7	9	18	-1	3	45	-30	2	2	40	-28	3	1	108	107					-2	6	93	-86	-1	2	157	162	-2	1	13	23
1	8	52	55	-1	4	34	32	2	3	100	-108	3	2	31	-26	0	0	30	17	-2	7	5	6	-1	3	87	70	-2	2	11	24
1	9	18	28	-1	5	79	-79	2	4	91	61	3	3	36	26	0	1	12	11	3	1	25	-26	-1	4	39	-36	-2	3	82	88
-1	1	134	107	-1	6	10	-10	2	5	80	81	3	4	49	44	0	2	13	6	3	2	12	5	-1	5	71	47	-2	4	51	44
-1	2	129	-136	-1	7	9	-22	2	6	9	27	3	5	9	14	0	3	21	-42	3	3	32	-50	2	1	11	2	-2	5	69	91
-1	3	100	-75	-1	8	22	34	2	7	8	2	3	6	34	40	0	4	187	-196	3	4	41	-34	2	2	82	-83	3	1	37	40
-1	4	293	-280	-1	9	5	-14	-2	1	49	-44	3	7	5	-2	0	5	44	-37	3	5	25	25	2	3	11	26	3	2	71	78
-1	5	101	103	2	0	192	191	-2	2	111	-103	-3	0	305	277	0	6	151	159	-3	1	82	-81	2	4	69	67	-3	1	34	31
-1	6	58	-60	2	1	111	-102	-2	3	100	83	-3	1	280	293	0	7	32	-36	-3	2	42	34	-2	1	49	-43	-3	2	62	39
-1	7	32	-39	2	2	61	-49	-2	4	87	-90	-3	2	273	-294	0	8	3	-34	-3	3	65	-58	-2	2	42	22	-3	3	11	56
-1	8	104	119	2	3	120	117	-2	5	21	-26	-3	3	87	70	1	0	33	39	-3	4	13	6	-2	3	75	68	-3	4	66	-62
-1	9	5	40	2	4	117	124	-2	6	24	-15	-3	4	14	-6	1	1	129	-148	-3	5	43	42	-2	4	101	81	-4	1	84	90
2	1	57	48	2	5	41	38	-2	8	57	-58	-3	5	13	1	1	2	111	-128	-3	6	6	1	-2	5	10	7	-4	2	68	-72
2	2	366	-380	2	6	9	15	3	1	76	60	-3	6	38	-32	1	3	41	40	4	1	7	3	-2	6	37	-34				
2	3	168	162	2	7	8	1	3	2	41	-20	-3	7	22	17	1	4	55	-60	4	3	31	-40	3	1	10	4		L = 26		
2	4	168	147	2	8	22	-26	3	3	13	18	4	0	25	3	1	5	83	73	-4	1	54	41	3	2	11	11				
2	5	14	23	-2	0	281	-291	3	4	21	18	4	1	11	24	-1	6	128	-144	-4	2	14	4	3	3	47	-52	0	0	66	69
2	6	17	-9	-2	1	338	-359	3	5	10	10	4	2	65	-44	1	7	6	-4	-4	4	97	93	3	4	71	-88	0	1	56	48
2	7	9	47	-2	2	171	167	3	6	9	5	4	3	11	20	-1	0	69	-53	-4	5	77	-65	-3	1	100	130	0	2	10	14
2	8	7	12	-2	3	87	81	3	7	18	-11	4	4	71	58	-1	1	26	-10	-5	1	49	57	-3	2	109	94	0	3	29	15
-2	1	58	-54	-2	4	60	-42	-3	1	320	-372	-4	0	98	90	-1	2	319	-298	-5	2	61	-61	-3	3	58	60	0	5	20	-27
-2	2	51	-26	-2	5	107	98	-3	2	253	261	-4	1	62	60	-1	3	130	-120					-3	4	14	11	1	0	34	30
-2	3	119	-113	-2	6	86	79	-3	3	139	123	-4	2	87	73	-1	4	203	197		L = 22			-3	5	68	27	1	1	23	9
-2	4	33	20	-2	7	27	-26	-3	4	52	-44	-4	4	249	-227	-1	5	44	42					4	1	31	-51	1	2	51	55
-2	5	14	-3	-2	8	128	-132	-3	5	115	-123	-4	5	87	-74	2	0	79	-76	0	0	122	-142	-4	1	79	86	1	3	26	31
-2	6	116	102	3	0	308	-326	-3	6	78	-92	5	2	19	22	2	1	47	-45	0	1	91	94	-4	2	12	-15	-1	0	28	10
-2	7	9	7	3	1	71	-66	-3	7	8	1	5	3	9	-9	2	2	82	65	0	2	44	50	-4	3	33	-28	-1	1	68	76
-2	8	87	-68	3	2	174	145	4	1	30	36	-5	0	72	-64	2	3	13	-7	0	3	11	21	-4	4	125	-135	-1	2	14	26
-2	9	5	-20	3	3	13	11	4	2	92	82	-5	1	42	-49	2	4	61	-58	0	4	23	-25					-1	3	51	-44
3	1	49	-35	3	4	72	59	4	3	48	-40	-5	2	78	-63	2	6	7	-7	0	6	6	-30		L = 24			-1	4	94	92
3	2	225	201	3	5	10	11	4	4	35	35	-5	4	12	15	2	7	5	-2	1	0	207	216					2	0	15	14
3	3	63	64	3	6	33	38	4	6	35	-40	-5	5	97	94	-2	0	227	-250	1	1	69	-84	0	1	29	-35	2	1	41	-49
3	4	14	-18	3	7	41	-46	-4	1	77	87	-6	0	43	44	-2	1	39	39	1	2	88	-85	0	2	29	-6	2	1	16	12
3	5	23	3	-3	0	13	2	-4	2	49	-30					-2	2	91	85	1	3	41	-35	0	3	36	-27	-2	0	13	-19
3	6	10	-11	-3	1	34	35	-4	4	102	81		L = 19			-2	3	107	103	1	4	44	-47	0	4	59	58	-2	1	55	-53
3	7	20	24	-3	2	241	-259	-4	5	13	19					-2	4	47	-1	1	5	8	-4	0	5	34	14	-2	2	78	65
3	8	5	9	-3	3	131	-121	-4	6	84	-73	0	1	65	-76	-2	5	13	12	1	6	6	-1	0	6	26	32	-2	3	90	101
-3	1	12	7	-3	4	178	161	-4	7	6	6	0	2	13	-8	-2	6	8	-13	-1	0	149	-126	1	0	63	67	-2	4	71	53
-3	2	31	31	-3	5	102	-93	5	2	24	-22	0	3	75	-88	-2	7	77	81	-1	1	93	-98	1	1	49	-57	3	0	59	-71
-3	3	54	49	-3	6	105	-120	5	3	8	5	0	4	224	215	3	0	63	-49	-1	2	17	-9	1	2	21	-26	3	1	5	51
-3	4	35	42	-3	7	37	-50	5	4	49	44	0	5	141	-139	3	1	53	48	-1	3	16	10	1	3	11	-2	-3	0	110	114
-3	5	39	39	-3	8	21	20	-5	1	76	-78	0	6	200	-207	3	2	69	-67	2	1	127	131	1	5	42	47	-3	3	55	-17
-3	6	162	-171	4	0	139	154	-5	2	44	-44	0	7	38	53	3	3	21	6	-1	5	102	87	-1	0	31	30				
-3	7	35	-42	4	1	31	-17	-5	4	96	-108	0	8	26	-30	3	4	12	9	2	0	69	-56	-1	1	14	14		L = 27		
-3	8	19	-22	4	2	77	-69	-5	5	109	-98	1	1	41	-29	3	5	29	-30	2	1	31	34	-1	2	79	84				
4	1	67	77	4	3	62	53	-6	1	28	-21	1	2	69	-66	3	6	6	-19	2	2	10	14	-1	3	44	-24	0	1	37	-32
4	2	170	178	4	4	69	61					1	3	33	-20	-3	0	327	333	2	3	47	-47	-1	4	14	-8	0	2	64	-61
4	3	70	70	4	6	6	-10		L = 18			1	4	51	44	-3	1	78	-70	2	4	55	-50	-1	5	91	76	0	3	84	100
4	4	47	-30	-4	0	131	-124					1	5	90	-79	-3	2	113	-114	2	6	34	-36	2	0	11	-8	0	4	47	38
4	5	45	-40	-4	1	14	8	0	0	36	-39	1	6	52	-66	-3	3	22	-23	-2	0	16	26	2	1	58	45	1	1	30	28
4	6	6	-16	-4	2	137	141	0	1	29	13	-1	1	42	-19	-3	4	82	-71	-2	1	46	49	2	2	27	25	1	2	6	2
-4	1	55	-58	-4	4	331	-311	0	2	13	24	-1	2	358	-329	-3	5	12	-11	-2	2	41	25	2	3	10	7	1	3	50	-50
-4	2	137	150	-4	5	80	-70	0	3	55	-55	-1	3	33	-30	-3	6	22	19	-2	3	13	11	2	4	37	31	-1	1	11	23
-4	3	142	-130	-4	6	58	38	0	4	362	-416	-1	4	33	80	4	0	101	-99	-2	4	39	24	-2	0	166	139	-1	2	12	-27
-4	4	14	-15	-4	7	59	25	0	5	116	129	-1	5	18	-13	4	1	20	-30	-2	5	56	-45	-2	1	11	1	-1	4	62	49
-4	5	22	14	5	0	57	-19	0	6	80	72	2	1	106	-113	4	2	11	12	-2	6	36	38	-2	2	12	-17	2	1	31	44
-4	6	106	-87	5	2	105	124	0	7	7	7	2	2	61	-54	4	3	20	1	3	0	35	-36	-2	3	11	27	2	2	18	-16
-4	7	55	-50	5	3	17	-21	0	8	5	-4	2	3	74	62	-4	0	15	-4	3	1	11	3	-2	4	93	84	-2	1	78	85
5	1	10	18	5	4	80	-97	1	0	32	11	2	4	117	-110	-4	1	67	-47	3	2	34	-35	-2	5	35	46	-2	2	34	19
5	2	76	-76	-5	0	100	96	1	1	31	50	2	5	8	-12	-4	2	41	-40	3	3	41	-44	3	0	8	8	-2	3	66	-61
5	3	11	11	-5	1	83	-85	1	2	66	80	2	6	6	-12	-4	4	72	-51	3	4	49	48	3	1	9	-1				
5	4	45	83	-5	2	129	-107	1	3	135	-132	-2	1	234	-244	-4	5	79	65	3	5	6	-21	3	2	37	42		L = 28		
-5	1	14	21	-5	3	53	-60	1	4	46	28	-2	2	307	298	-5	0	83	-57	-3	0	100	-100	3	3	26	-27				
-5	2	165	-139	-5	4	14	-2	1	5	14	-16	-2	3	101	-99	-5	1	11	3	-3	1	63	53	-3	0	85	67	0	0	45	51
-5	3	14	-21	-5	5	74	55	1	6	217	-216	-2	4	38	-36	-5	2	125	125	-3	2	128	124	-3	1	63	72	0	1	30	41
-5	4	14	-21	-6	0	188	-186	1	7	102	105	-2	5	55	49					-3	3	117	114	-3	2	135	143	0	2	39	52
-5	5	98	-87	-6	1	35	37	1	8	73	79	-2	6	43	-48		L = 21			-3	4	70	-38	-3	3	10	16	0	3	45	-67
-6	1	57	-54					-1	0	93	65	-2	7	63	-63					-3	5	78	71	-3	4	12	-2	1	0	42	-18
-6	2	103	-109		L = 17			-1	1	52	45	3	1	66	-67	0	1	100	111	-3	6	36	-31	-4	0	131	136	1	1	5	10
-6	4	22	48					-1	2	209	-184	3	2	26	-21	0	2	112	125	4	1	6	-14	-4	1	10	-9	1	2	22	-15
				0	1	51	-44	-1	3	159	-160	3	3	12	-3	0	3	118	-137	4	3	38	41	-4	2	114	-95	-1	0	132	128
	L = 16			0	2	12	7	-1	4	155	153	3	4	13	2	0	5	38	-1	-4	0	257	248	-4	3	42	-36	-1	1	73	91
				0	3	47	59	-1	5	99	88	3	5	27	30	0	6	80	-100	-4	1	56	50					-1	2	80	-79
0	0	218	235	0	4	175	185	-1	6	83	-77	3	6	46	39	1	1	44	-40	-4	2	83	74		L = 25			-2	0	115	-137
0	1	114	-105	0	5	123	-128	2	0	118	-115	-3	1	78	71	1	2	34	-19	-4	3	12	-3					-2	1	115	-137
0	2	126	114	0	6	8	13	2	1	44	31	3	2	263	283	1	3	88	85	-4	4	11	2	0	1	66	64	-2	2	128	125
0	3	29	-27	0	7	8	-14	2	2	103	-92	-3	3	13	-4	1	4	20	-24	-5	0	54	-49	0	2	11	16				
0	4	47	-40	0	8	32	45	2	3	13	5	-3	4	99	-90	1	5	9	-6	-5	1	26	25	0	3	27	29		L = 29		
0	5	117	107	1	1	72	-73	2	4	11	-13	-3	5	13	-13	-1	1	98	-116					0	4	57	-55				
0	6	38	-40	1	3	13	-23	2	5	13	-9	-3	6	8	1	-1	2	78	-57		L = 23			0	5	22	-19	-1	1	34	31
0	7	8	16	1	4	192	-190	2	6	69	65	-3	7	6	-14	-1	3	16	-3					1	1	45	51				
0	8	6	-12	1	5	120	117	2	7	7	2	4	1	9	9	-1	4	82	55	0	1	29	11	1	2	18	-20				

Sundaralingam, 1970) and 5-methyluridine (Hunt & Subramanian, 1969). Of the nitrogen–carbon bond distances, the N(1)–carbon bond lengths are somewhat longer than the values around the N(2) atom. The difference between the bond distances of the two nitrogen atoms may be explained on the basis that the substitution of the phenyl group at the N(1) nitrogen atom will tend to prevent this nitrogen atom from forming a double bond with adjacent carbon atoms in the ring. The oxygen–carbon bond lengths of 1·201 Å [O(1)–C(1)] and 1·213 Å [O(2)–C(8)] indicate double-bonded character. These values may be compared with 1·209 and 1·211 Å for 10-methylisoalloxazine hydrobromide dihydrate (Trus & Fritchie, 1969), and 1·206 and 1·197 Å for aflatoxin B_2 (Van Soest & Peerdeman, 1970). The apparent bond distances and angles involving the hydrogen atoms are listed in Table 5. All the values except those related to H(4) are reasonable. Fig. 5 shows the shapes and relative magnitudes of the thermal ellipsoids with a probability of 50 per cent for atoms other than hydrogen (Johnson, 1965).

Molecular arrangement

The molecular arrangements in the crystal viewed along the *a* and the *c* axes are illustrated in Figs. 6 and 7. The same symbols in both Figures designate the same molecules. The quinazoline rings are superimposed at intervals of 3·5 Å along the *b* axis, with their long axes approximately parallel to the [001] direction. The molecules are placed in pairs around a centre of sym-

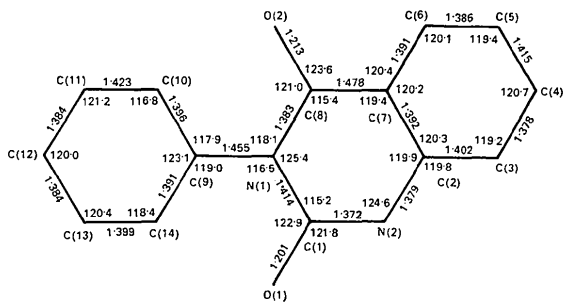

Fig. 4. Bond lengths (Å) and angles (°) of the molecule.

Table 4. *Intramolecular bond distances and angles with their standard deviations*

C(1)–N(2)	1·372 (5) Å	C(4)—C(5)	1·415 (5) Å
N(2)–C(2)	1·379 (5)	C(5)—C(6)	1·386 (5)
C(2)–C(7)	1·392 (5)	C(6)—C(7)	1·391 (6)
C(7)–C(8)	1·478 (5)	N(1)—C(9)	1·455 (5)
C(8)–N(1)	1·393 (5)	C(9)—C(10)	1·396 (5)
N(1)–C(1)	1·414 (5)	C(10)–C(11)	1·423 (5)
C(1)–O(1)	1·201 (4)	C(11)–C(12)	1·384 (5)
C(8)–O(2)	1·213 (5)	C(12)–C(13)	1·384 (5)
C(2)–C(3)	1·402 (5)	C(13)–C(14)	1·399 (5)
C(3)–C(4)	1·378 (5)	C(14)–C(9)	1·391 (5)
	N(1)—C(1)—N(2)	115·2 (4)°	
	C(1)—N(2)—C(2)	124·6 (4)	
	N(2)—C(2)—C(7)	119·9 (4)	
	C(2)—C(7)—C(8)	119·4 (4)	
	C(7)—C(8)—N(1)	115·4 (4)	
	C(8)—N(1)—C(1)	125·4 (5)	
	N(1)—C(1)—O(1)	122·9 (4)	
	N(2)—C(1)—O(1)	121·8 (4)	
	C(7)—C(8)—O(2)	123·6 (4)	
	N(1)—C(8)—O(2)	121·0 (4)	
	N(2)—C(2)—C(3)	119·8 (4)	
	C(2)—C(3)—C(4)	119·2 (4)	
	C(3)—C(4)—C(5)	120·7 (4)	
	C(4)—C(5)—C(6)	119·4 (4)	
	C(5)—C(6)—C(7)	120·1 (5)	
	C(6)—C(7)—C(2)	120·2 (4)	
	C(7)—C(2)—C(3)	120·3 (4)	
	C(6)—C(7)—C(8)	120·4 (4)	
	C(1)—N(1)—C(9)	116·5 (4)	
	C(8)—N(1)—C(9)	118·1 (5)	
	N(1)—C(9)—C(10)	117·9 (4)	
	N(1)—C(9)—C(14)	119·0 (4)	
	C(9)—C(10)–C(11)	116·8 (4)	
	C(10)–C(11)–C(12)	121·2 (4)	
	C(11)–C(12)–C(13)	120·0 (4)	
	C(12)–C(13)–C(14)	120·4 (4)	
	C(13)–C(14)–C(9)	118·4 (4)	
	C(14)–C(9)—C(10)	123·1 (4)	

Table 5. *Bond distances and angles involving the hydrogen atoms*

H(1)–N(2)	0·91 Å	H(6)—C(10)	1·00 Å
H(2)–C(3)	0·97	H(7)—C(11)	1·11
H(3)–C(4)	0·90	H(8)—C(12)	0·93
H(4)–C(5)	1·19	H(9)—C(13)	1·05
H(5)–C(6)	0·94	H(10)–C(14)	1·01
	H(1)—N(2)—C(1)	113°	
	H(1)—N(2)—C(2)	118	
	H(2)—C(3)—C(2)	131	
	H(2)—C(3)—C(4)	108	
	H(3)—C(4)—C(3)	113	
	H(3)—C(4)—C(5)	127	
	H(4)—C(5)—C(4)	122	
	H(4)—C(5)—C(6)	108	
	H(5)—C(6)—C(5)	123	
	H(5)—C(6)—C(7)	116	
	H(6)—C(10)–C(9)	119	
	H(6)—C(10)–C(11)	125	
	H(7)—C(11)–C(10)	110	
	H(7)—C(11)–C(12)	129	
	H(8)—C(12)–C(11)	114	
	H(8)—C(12)–C(13)	126	
	H(9)—C(13)–C(12)	123	
	H(9)—C(13)–C(14)	114	
	H(10)–C(14)–C(13)	120	
	H(10)–C(14)–C(9)	120	

metry, connected by two C=O···H–N hydrogen bonds with a length of 2·821 Å. The oxygen atom O(1) forms a hydrogen bond with the hydrogen atom at N(2); O(2) is not hydrogen bonded at all. An infrared spectrum also showed the presence of the two kinds of carbonyl group; an absorption band at 1650 cm^{-1} is assigned to the hydrogen-bonded carbonyl, while an absorption band at 1730 cm^{-1} is assigned to the free carbonyl group. The quinazoline ring atoms of the molecule are nearly coplanar. The best plane through the ten atoms of the quinazoline ring, as calculated by the least-squares method, is defined with respect to the crystallographic axes by the equation

$$0{\cdot}9841x - 1{\cdot}5093y + 0{\cdot}1000z = -0{\cdot}3147;$$

the distance from this plane to the origin is 0·3147 Å. The average deviation of the ten ring atoms from the plane is 0·03 Å, with the maximum deviation of 0·07 Å for atom C(8); the departures from this plane of the two oxygen atoms attached to the ring are as follows:

O(1), 0·173 Å; O(2), −0·220 Å.

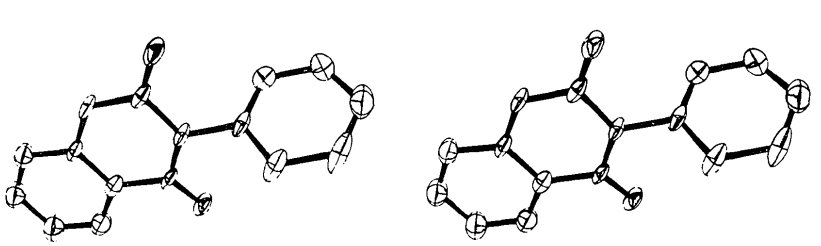

Fig. 5. A stereoscopic pair of the molecule and the shape and relative magnitude of the thermal ellipsoids with the probability of 50 per cent for atoms other than hydrogen.

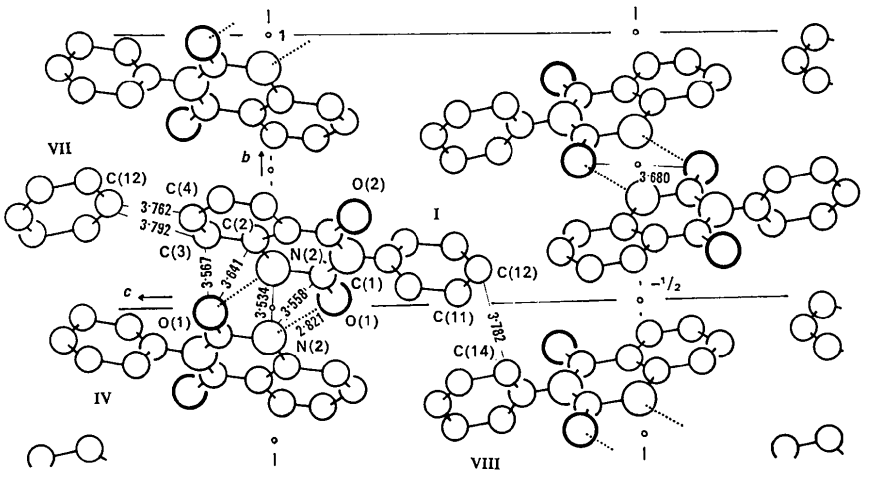

Fig. 6. The crystal structure projected along the *a* axis. The intermolecular short distances are shown by solid lines and hydrogen bonds are shown by dotted lines.

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

i	x	y	z	vi	$1-x$	$1-y$	$-z$
ii	$1+x$	y	z	vii	x	$\frac{1}{2}-y$	$\frac{1}{2}+z$
iii	$-1+x$	y	z	viii	$-x$	$-\frac{1}{2}+y$	$-\frac{1}{2}-z$
iv	$-x$	$-y$	$-z$	ix	$1-x$	$-\frac{1}{2}+y$	$-\frac{1}{2}-z$
v	$1-x$	$-y$	$-z$				

C(1^{i})–C(2^{v})	3·531 Å	C(5^{i})—N(1^{vi})	3·795 Å
C(1^{i})–C(3^{v})	3·601	C(5^{i})—O(1^{v})	3·556
C(1^{i})–N(2^{iv})	3·558	C(5^{i})—O(2^{vi})	3·763
C(1^{i})–O(1^{iv})	3·691	C(6^{i})—C(6^{vi})	3·789
C(1^{i})–O(2^{iii})	3·738	C(6^{i})—C(7^{vi})	3·520
C(2^{i})–C(6^{vi})	3·628	C(6^{i})—N(2^{ii})	3·405
C(2^{i})–N(2^{v})	3·578	C(6^{i})—O(1^{v})	3·729
C(2^{i})–O(1^{iv})	3·641	C(7^{i})—C(7^{vi})	3·781
C(3^{i})–C(10^{v})	3·521	C(7^{i})—N(2^{v})	3·634
C(3^{i})–C(12^{vii})	3·792	C(8^{i})—O(1^{ii})	3·545
C(3^{i})–N(1^{v})	3·675	C(11^{i})–O(2^{ix})	3·601
C(3^{i})–O(1^{iv})	3·567	C(12^{i})–C(14^{viii})	3·782
C(3^{i})–O(1^{v})	3·700	C(12^{i})–O(2^{ix})	3·452
C(3^{i})–O(2^{vi})	3·715	C(14^{i})–O(2^{iii})	3·350
C(4^{i})–C(8^{vi})	3·555	N(2^{i})—N(2^{iv})	3·534
C(4^{i})–C(12^{vii})	3·762	N(2^{i})—N(2^{v})	3·731
C(4^{i})–O(1^{v})	3·547	N(2^{i})—O(1^{iv})	2·821*
C(4^{i})–O(2^{vi})	3·355	O(1^{i})—O(1^{iv})	3·680
C(5^{i})–C(7^{vi})	3·619	O(1^{i})—O(2^{iii})	3·423
C(5^{i})–C(8^{vi})	3·483		

* Hydrogen bonding.

In terms of the standard deviations, the deviations of these two oxygen atoms are probably significant. The equation for the best plane representing the benzene ring coordinated to atom N(1) is

$$0{\cdot}9400x+1{\cdot}4763y-0{\cdot}4057z=4{\cdot}9630\,.$$

The average displacement of the atom from the mean plane is 0·01 Å, with the maximum deviation of 0·03 Å for atom C(9). The benzene ring is rotated by 65·0° from the quinazoline ring because of the steric effect of the two carbonyl groups, the distance O(1)–C(14), O(2)–C(10) being 3·059 and 2·990 Å, respectively. This feature of the benzene ring may be compared with those in phenyl substituted isoxazolins. The dihedral angle between phenyl plane and isoxazolin plane is 50·4° for *N*-methyl-3-phenyl-4-bromoisoxazolin-5-one (Sabelli & Zanazzi, 1969*b*), whereas the angles are slightly twisted by 11 to 14° for *N*-methyl-4-phenylisox-

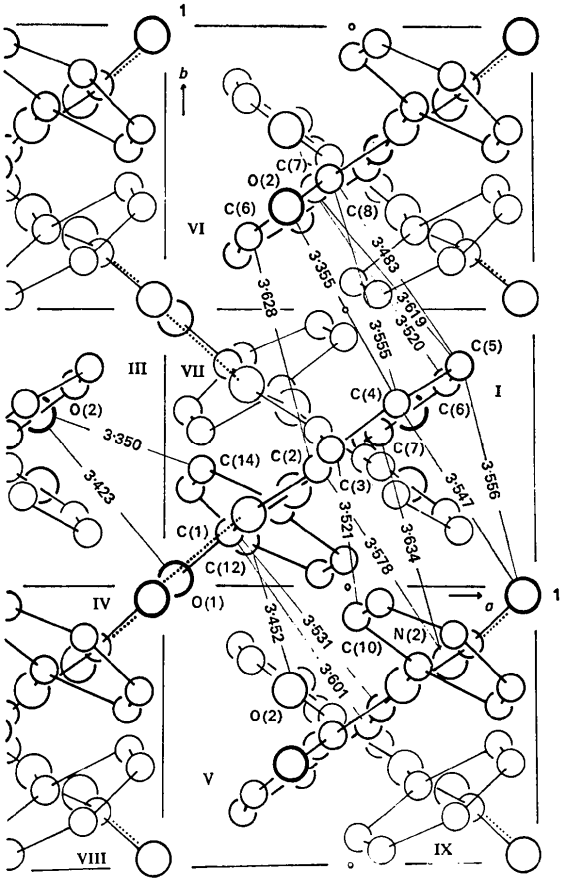

Fig. 7. The crystal structure projected along the *c* axis. The intermolecular short distances are shown by solid lines and hydrogen bonds are shown by dotted lines.

azolin-5-one (Sabelli & Zanazzi, 1969*a*) and by 2·45° for 3-phenylisoxazolin-5-one (Cannas, Biagini & Marongiu, 1969). The intermolecular distances less than 3·8 Å are listed in Table 6 and shown in Figs. 6 and 7. The shortest intermolecular distances are as follows:

$C(14^{i})\cdots O(2^{iii})$, 3·350; $C(4^{i})\cdots O(2^{vi})$, 3·355; $C(6^{i})\cdots N(2^{ii})$, 3·405; $O(1^{i})\cdots O(2^{iii})$, 3·423; $C(12^{i})\cdots O(2^{ix})$, 3·452 Å.

Computation

The main part of the calculations was performed on an IBM 7040 computer with the use of the program *ERBR* 1 (Van den Hende, 1961) for structure factor and least-squares refinement and the program *ERFR* 2 (Sly, Shoemaker & Van den Hende, 1962) for Fourier summation. The final block-diagonal least-squares refinements were carried out with the program *HBLS* (Ashida, 1964). Thermal ellipsoids were drawn by the CDC 3600 computer at C. Itoh Electronic Computing Service Co. Ltd. using the program *ORTEP* (Johnson, 1965).

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The Crystal Structure of Cs_2MnBr_4

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The crystal structure of Cs_2MnBr_4, determined from Weissenberg data, is orthorhombic with $a=10{\cdot}150$ (23), $b=7{\cdot}806$ (11) and $c=13{\cdot}70$ (8) Å. The space group is *Pnma* and $Z=4$. The structure is isomorphous with that of Cs_2ZnBr_4.

Introduction

The material examined in this work was prepared by heating a mixture, consisting of stoichiometric amounts of CsBr and $MnBr_2$, in a sealed evacuated silica tube until molten at about 650 °C. The specimen was then cooled slowly (10 °C per hour) to room temperature and single crystals suitable for X-ray study were selected from the yellow crystalline mass. Because the material was very unstable in the presence of water vapour, each crystal was sealed in a Lindemann glass tube containing P_2O_5.

The space lattice and unit-cell dimensions were determined from rotation and Weissenberg photo-