ACTA CHEMICA SCANDINAVICA 27 (1973) 945–969

Crystal Structure of Some Benzoxazoline Derivatives

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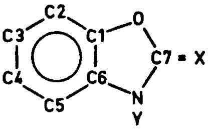
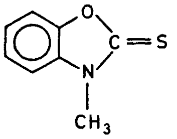
The compounds investigated (six in all) are of the type with $X = S$, O, benzylimino, and $Y = H$, CH_3: (I) 3-methyl-benzoxazoline-2-thione; (II) benzoxazoline-2-thione; (III) 3-methyl-benzoxazoline-2-one; (IV) benzoxazoline-2-one; (V) 2-benzylimino-3-methyl-benzoxazoline; and (VI) 2-benzylimino-benzoxazoline. Neither methylation nor substitution of S with O changes the geometry significantly for (I) – (IV). For the methylated compound (V) there are very small changes also on substitution with $N-CH_2-C_6H_5$. The molecules of (VI) form dimers with N···H···N bonds of length 2.933 Å. Some averaged bond distances and angles for (I) – (V) with corresponding values for (VI) in parentheses are: O – C7: 1.383(1.375) Å; N – C7: 1.349(1.310) Å; C1 – O – C7: 107.4(104.0)°; O – C7 – N: 107.8(114.2)°; C7 – N – C1: 109.9(105.1)°. The differences are probably related to the hydrogen bond formation.

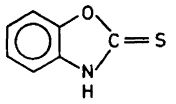


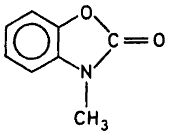
The interactions of benzoxazolone, benzoxazolethione, and their derivatives with fatty, aromatic, and alkylaromatic amines have been studied by Simov *et al.*[1–4] The main features are: (1) the heteroatomic ring is opened and asymmetric di- or tri-substituted ureas or thioureas are obtained; (2) the products are derivatives of 2-aminobenzoxazole;[5] and (3) substitution of H in NH by CH_3 reduces the interaction rate in the case of benzoxazolone, while it has the opposite effect for benzoxazolethione.

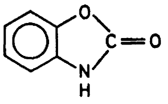
Infrared stretching frequencies of C = N in iminobenzoxazolines have been determined to lie in the interval 1717 – 1745 cm^{-1}.[6] This is considerably higher than reported values (1670 – 1690 cm^{-1}) for azomethine groups in non-conjugated positions to conjugated systems.[7,8]

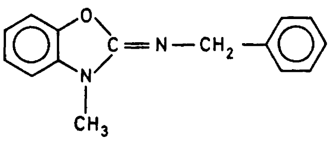
Hoping to elucidate these and some other characteristics, X-ray crystal structure analyses of the following benzoxazoline derivatives have been carried out:

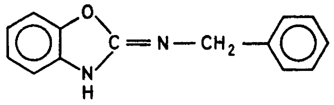

(I)


(II)


(III)


(IV)


(V)


(VI)

(I) 3-methyl-benzoxazoline-2-thione, (II) benzoxazoline-2-thione, (III) 3-methyl-benzoxazoline-2-one, (IV) benzoxazoline-2-one, (V) 2-benzylimino-3-methyl-benzoxazoline, and (VI) 2-benzylimino-benzoxazoline. The crystal structure determination of (I) (based on film data) has been presented earlier.[9] For comparison some results will be included in this paper.

For the compounds (II)–(VI) the intensities have been measured on an automatic four circle diffractometer with a highly orientated graphite crystal monochromator. The radiation used was Mo$K\alpha$ and $2\theta_{\max}$ ranged from 45° to 50°. No corrections for absorption or secondary extinction effects were carried out.

The phase problems for (III)–(VI) were solved by direct methods [10]* while the solution for (II) was obtained from the Patterson function. All structures have been refined by full-matrix least squares technique with weights calculated from the standard deviations in intensities, $\sigma(I)$, taken as

$$\sigma(I) = [C_{\rm T} + (0.02C_{\rm N})^2]^{\frac{1}{2}}$$

where $C_{\rm T}$ is the total number of counts and $C_{\rm N}$ the net count (peak minus background). Anisotropic temperature factors were introduced for all non-hydrogen atoms, the expression for the vibration being:

$$\exp - (B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl)$$

Crystal data and final R-values are given in Table 1. Methyl hydrogens were localized in difference Fourier maps; other H-positions were calculated. Refinements of isotropic thermal parameters for hydrogens gave reasonable results for (II) and (IV) only. Final fractional coordinates and thermal parameters with estimated standard deviations are given in Tables 2 and 3. A comparison between observed and calculated structure factors is presented in Table 4.

The principal axes of the thermal vibration ellipsoids were calculated from the thermal parameters of Table 2.

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* All programs used are included in this reference.

Table 1. Crystal data and final R-values.

Compound	Space group	Cell dimensions	Z	ϱ_{calc}	ϱ_{obs}	Observed reflections	R %	R_w %
I	$P2_1/c$	a = 9.24 Å b = 6.90 c = 12.86 β = 99.0°	4	1.35	1.34	674	7.7	11.3
II	$P2_1$	a = 8.573(3) Å b = 9.039(3) c = 4.353(2) β = 90.00 (3)°	2	1.49	1.49	545	3.2	3.7
III	$P2_1/c$	a = 5.716(1) Å b = 4.340(1) c = 29.506(4) β = 105.00 (1)°	4	1.40	1.37	912	3.3	3.8
IV	$P2_12_12_1$	a = 4.457(2) Å b = 6.654(3) c = 20.996(7)	4	1.44	1.43	506	2.7	3.0
V	$P2_1$	a = 14.267(5) Å b = 5.540(1) c = 8.946(3) β = 119.44 (3)°	2	1.28	1.25	957	5.1	5.5
VI	$P2_1/c$	a = 13.265(4) Å b = 7.556(3) c = 12.270(4) β = 111.96 (3)°	4	1.30	1.28	1016	3.8	4.6

Root mean square amplitudes, the corresponding B-values for the atomic anisotropic thermal vibration along the principal axes, as well as their components along the crystal axes are listed in Table 5.

By including all atoms in the molecules, the r.m.s. discrepancies between atomic anisotropic vibration tensor components calculated from the thermal parameters of Table 2, and those calculated from the rigid-body parameters obtained by analysis of librational, translational and screw motion[11] are:

(I)	(II)	(III)	(IV)	(V)	(VI)
0.0080	0.0031	0.0018	0.0021	0.0061	0.0051

The values for (III) and (IV) support the assumption of regarding these molecules as oscillating rigid bodies. However, the r.m.s. librational amplitudes are moderate:

(III) L1 = 5.4°, L2 = 3.7°, L3 = 3.4°
(IV) L1 = 6.0°, L2 = 4.8°, L3 = 3.7°

and no bond distance increased more than three times e.s.d. when corrected for libration. Uncorrected values for bond distances and angles are therefore presented in Table 6.

Table 2. Fractional atomic coordinates and anisotropic thermal vibration parameters with estimated standard deviations (multiplied by 10^5). For numbering of atoms, see Fig. 1.

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
(II)									
S	−16237	50000	−08389	01583	01048	05966	−00081	−00292	−00731
	10		20	15	13	59	39	40	78
O	05887	38945	27322	01553	00663	05978	−00020	00586	−00054
	53	32	100	59	39	219	72	170	146
N	07392	63036	22841	01584	00690	05384	−00012	00596	00352
	65	45	122	70	50	249	91	205	171
C1	18584	43555	44423	01211	00879	04555	00061	01211	00025
	65	62	131	85	59	323	104	270	187
C2	28553	35168	61025	01641	01069	06811	00283	01043	00945
	77	73	152	99	73	364	153	310	269
C3	40512	42855	75835	01875	01564	05863	00666	01017	01427
	92	87	182	123	98	386	179	368	309
C4	41853	58117	73870	01309	01537	05866	−00031	−00121	00109
	87	85	175	86	87	359	146	294	291
C5	31454	66496	57007	01599	00986	06289	−00267	01136	−00372
	74	75	139	97	69	362	122	290	251
C6	19944	58849	41907	01412	00813	04438	00017	01202	−00001
	68	61	128	94	60	306	106	286	203
C7	−00869	51069	14042	01497	00832	04542	−00021	01479	−00262
	36	76	70	48	47	170	145	150	278
(III)									
O1	23850	05901	43900	05114	09109	00216	−01027	00816	00204
	24	35	5	58	106	2	124	20	26
O2	16386	30043	36851	03374	07063	00197	−01196	00319	−00208
	19	29	4	40	85	2	97	16	22
N	51493	39313	41963	03251	06574	00156	00060	00325	−00310
	23	33	4	49	97	2	113	16	26
C1	29478	50369	34816	03236	05289	00170	00222	00345	−00355
	28	40	6	59	102	3	133	22	28
C2	22918	62688	30432	03876	06877	00183	00522	00137	−00337
	36	48	7	68	133	3	162	24	34
C3	39747	82174	29206	05089	06498	00182	01223	00531	−00108
	37	46	7	80	127	3	176	27	34

Table 2. Continued.

C4	61710	88316	32345	04609	06225	00212	-00302	00813	-00178
	37	46	7	80	126	4	161	29	25
C5	68101	75495	36789	03384	06530	00191	-00586	00427	-00498
	32	45	7	60	119	3	149	23	34
C6	51339	56207	37960	03103	05193	00158	00679	00375	-00420
	28	38	5	58	101	3	124	20	27
C7	30472	23409	41291	03767	06593	00178	00448	00522	-00302
	32	46	7	65	120	3	155	24	33
CM	70878	37979	46198	04272	09934	00168	00525	00281	-00309
	39	67	7	77	184	3	203	26	40
					(IV)				
O1	48036	38625	20099	08708	03794	00311	-03531	-00542	-00466
	36	30	10	116	57	6	144	39	30
O2	14726	31072	12387	05823	02158	00254	-00718	-00272	00108
	28	21	8	84	34	4	87	28	23
N	25352	07379	19347	05761	02560	00204	00964	-00282	00143
	39	31	10	103	49	5	121	38	28
C1	-01331	13934	10816	03983	02055	00215	00248	00120	-00007
	37	28	11	90	48	6	109	34	27
C2	-20513	11422	05757	04846	03192	00239	00247	-00250	00171
	49	47	12	111	74	6	156	44	40
C3	-33607	-07291	05194	04761	03868	00284	-01147	-00111	-00568
	50	49	15	121	88	8	169	48	46
C4	-27438	-22479	09440	05382	02672	00372	-01692	00579	-00618
	51	44	14	138	66	9	169	56	43
C5	-07933	-19796	14491	05683	02171	00310	00687	00684	00063
	47	37	14	122	57	8	141	49	41
C6	05126	-00998	15064	03841	02045	00214	00802	00260	-00032
	38	31	11	91	47	6	109	38	29
C7	31358	26487	17668	05564	02608	00215	-00526	-00104	-00151
	48	37	11	117	63	6	148	41	33
					(V)				
O	23120	71900	48112	00632	03690	01474	00836	00920	01137
	20		30	21	134	52	109	55	157
N1	19308	75930	19240	00591	04741	01551	00116	01091	-00459
	25	93	41	25	195	64	131	67	201
N2	12481	101778	32170	00522	04132	01380	00587	00868	00639
	24	106	38	25	171	63	132	65	194

Table 2. Continued.

C1	19998	85614	58089	00516	03443	01310	−00154	00919	−00151
	30	103	46	29	193	73	148	77	226
C2	22753	81456	74840	00582	04188	01405	−00125	00772	00077
	33	116	52	31	215	77	160	80	232
C3	18751	98070	82012	00763	05196	01390	−00329	01073	−00781
	35	124	57	37	266	82	196	91	280
C4	12318	116716	72510	00764	04223	01800	00017	01413	−01053
	37	120	56	35	225	91	173	94	262
C5	09464	120543	55327	00610	04449	01940	00132	01193	00283
	34	126	55	31	217	90	168	87	269
C6	13480	104029	48421	00437	03112	01342	−00049	00678	00276
	29	100	45	28	171	78	140	75	222
C7	18308	82921	31832	00453	03229	01419	00057	00701	00092
	30	99	47	30	192	74	145	78	215
C8	26260	55334	21394	00705	04533	01970	−00689	01349	−01334
	39	124	69	35	238	96	178	95	275
C9	36952	62633	22746	00562	03655	01192	00262	00811	00201
	31	101	48	32	199	71	138	82	209
C10	41465	48115	15573	00621	03548	01672	00196	00864	−00277
	33	116	51	32	210	84	162	84	234
C11	51445	54041	17245	00742	04918	02317	01096	01506	00603
	38	129	63	38	249	107	192	107	210
C12	56738	74331	25964	00624	05759	02176	00325	01216	00957
	40	132	62	38	283	105	201	111	328
C13	52195	89143	32704	00696	03780	01997	−00300	00796	−00369
	37	122	55	36	220	93	171	97	271
C14	42286	83354	31261	00704	04150	01631	−00035	00983	−01005
	36	109	56	35	220	83	174	92	247
CM	05663	116275	17160	00588	04291	01697	00538	00754	01873
	40	129	59	30	217	80	158	83	256

(VI)

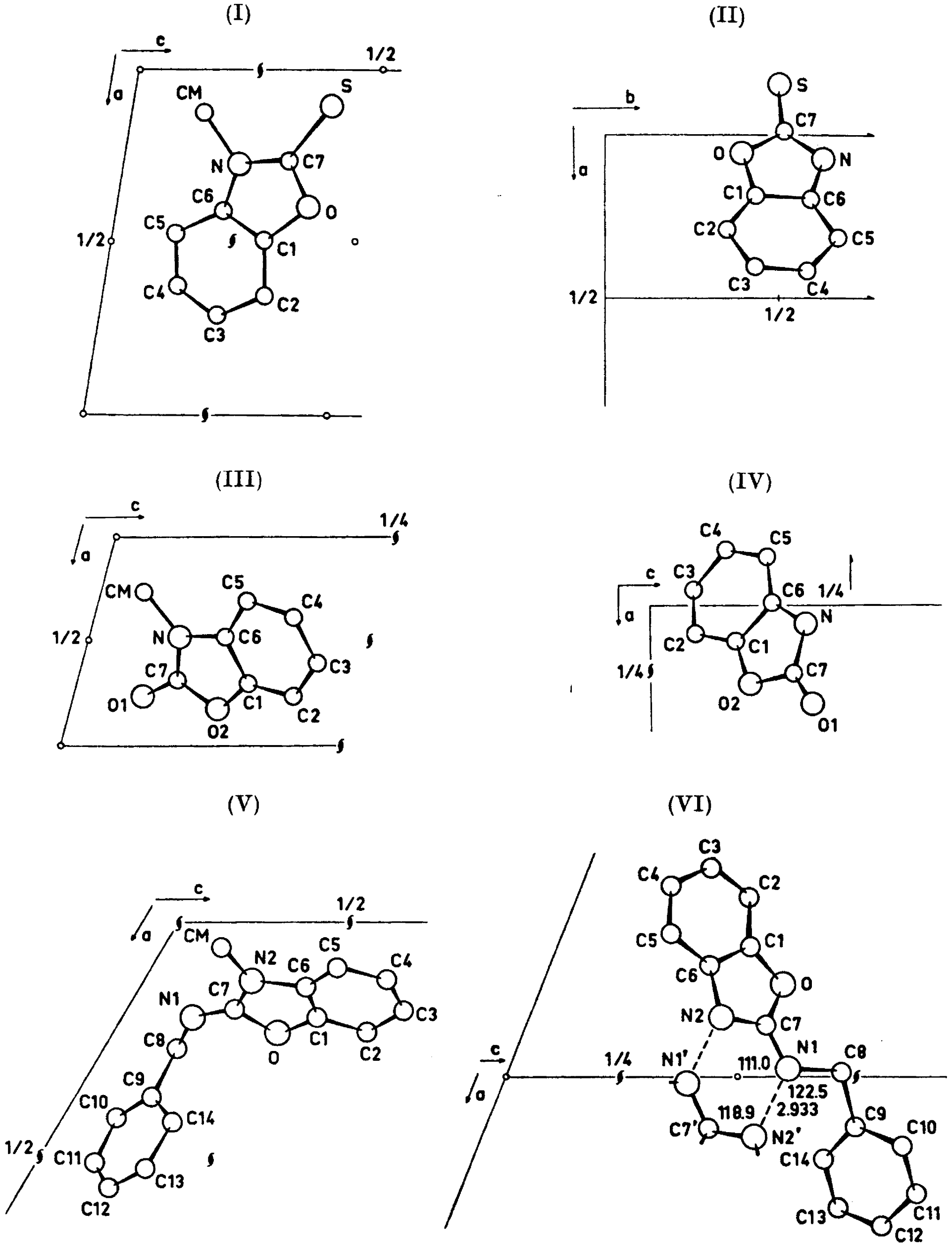
O	80232	23283	51889	00641	01888	00714	−00478	00536	00284
	13	22	13	15	44	17	53	28	46
N1	98300	31827	60403	00632	01980	00544	−00139	00216	00541
	16	28	16	19	54	19	54	32	55
N2	87039	40006	41039	00654	01353	00743	−00272	00587	00151
	16	27	17	19	47	22	50	33	53
C1	71998	26057	40993	00559	01582	00663	−00251	00451	00049
	20	33	21	20	62	24	60	39	65

Table 2. Continued.

C2	61464	20388	37215	00670	02394	00975	−00638	00758	00019
	22	43	26	26	76	30	73	47	79
C3	54822	24949	25919	00552	02542	00909	−00092	00384	−00216
	23	42	24	22	85	30	70	45	86
C4	58865	35198	19011	00694	01961	00768	00453	00307	00072
	22	38	25	25	72	27	69	43	73
C5	69555	40994	23031	00663	01635	00721	00135	00446	00160
	21	36	22	23	63	27	65	43	65
C6	76126	36343	34354	00506	01343	00672	−00141	00443	−00251
	18	31	20	21	56	24	56	37	61
C7	88988	32220	51161	00656	01235	00707	−00202	00708	00147
	20	32	21	22	54	26	58	41	61
C8	98988	24026	71608	00705	01659	00700	−00145	00538	00349
	22	40	22	23	62	25	64	41	67
C9	110656	21027	79414	00656	01228	00671	−00131	00530	00251
	20	32	20	22	53	25	59	38	60
C10	114644	26424	91017	00812	01892	00659	−00046	00546	00164
	24	37	22	25	68	25	69	41	70
C11	125247	23244	98301	00952	02456	00685	−00318	00371	00214
	25	43	25	30	82	26	81	48	79
C12	132214	14545	94109	00739	02194	01003	00118	00240	00616
	25	42	27	26	81	33	74	48	81
C13	128414	09183	82581	00770	01949	01162	00432	00737	00170
	24	41	29	26	78	34	74	51	83
C14	117802	12269	75326	00868	01703	00754	−00071	00626	−00049
	23	37	25	28	68	27	69	46	70

The molecules (I), (II), (III), and (IV) are planar to within 0.02 Å. By excluding CM in (V), the parts of the molecules (V) and (VI) separated by the N1 – C8-bond are also planar to within 0.02 Å, with angles between the planes of 89° and 117°, respectively. CM is out of the plane through O, N1, N2, C1,..., C7 by 0.14 Å. (For numbering of atoms, see Fig. 1.)

In the reactions mentioned above the opening of the heteroatomic ring occurs at the C7 – O bond. As mentioned above, the interaction rate is larger for (I) than for (II). The C7 – O distance of (I) (1.393 Å) seems to be somewhat longer than that of (II) (1.369 Å). However, the standard deviations are large, and the difference is not significant. The opposite effect for benzoxazolone, (IV) reacting faster than (III), is not at all reflected in the C – O distances (1.379 Å for (III) and 1.368 Å for (IV)). The bonds are equal within error limits. For the iminobenzoxazolines, however, the C – O bond distance of the 2-



(I)

(II)

(III)

(IV)

(V)

(VI)

c
a
1/2
CM
S
N
C7
C6
C5
O
C1
C4
C2
C3
b
C7
O
N
C1
C6
C2
C5
C3
C4
1/2
1/2
1/4
CM
C5
C4
N
C6
C3
C7
O1
C1
C2
O2
C4
C5
C3
C6 1/4
N
C2
C1
1/4
C7
O2
O1
CM
N2
C6
C5
C4
N1
C7
C3
C8
O
C1
C2
C9
C10
C14
C11
C13
C12
C3
C4
C2
C5
C1
C6
O
N2
C7
N1
C8
N1'
111.0
122.5
2.933
118.9
C7'
N2'
C9
C10
C14
C11
C13
C12

Fig. 1. (I) 3-Methyl-benzoxazoline-2-thione viewed along [010], (II) benzoxazoline-2-thione viewed along [001], (III) 3-methyl-benzoxazoline-2-one viewed along [010], (IV) benzoxazoline-2-one viewed along [010], (V) 2-benzylimino-3-methyl-benzoxazoline viewed along [010], and (VI) 2-benzylimino-benzoxazoline viewed along [010].

Table 3. Fractional atomic coordinates and isotropic thermal parameters, with estimated standard deviations, for hydrogen atoms. Hm and Hm,n are bonded to Cm, HM,n to CM and HN to N.

Atom	x	y	z	B(Å^2)
		(II)		
HN	.0502 47	.7207 54	.1734 91	3.7 1.0
H2	.2774 50	.2387 61	.6404 99	4.2 1.0
H3	.4885 65	.3825 67	.9016 120	5.3 1.4
H4	.5033 70	.6346 62	.8262 131	4.9 1.4
H5	.3242 50	.7666 65	.5368 102	3.9 1.1
		(III)		
H2	.0780 33	.5791 40	.2831 6	5.0
H3	.3657 32	.9193 42	.2603 7	5.0
H4	.7344 33	1.0100 43	.3136 6	5.0
H5	.8293 34	.7947 41	.3898 6	5.0
HM,1	.7347 33	.5759 47	.4765 6	5.0
HM,2	.8498 35	.3017 44	.4557 6	5.0
HM,3	.6671 32	.2370 47	.4851 6	5.0
		(IV)		
HN	.3331 49	.0064 38	.2227 15	4.3 0.6
H2	−.2432 52	.2131 42	.0294 14	4.6 0.7
H3	−.4630 60	−.0998 53	.0183 19	6.6 0.6
H4	−.3686 52	−.3553 41	.0910 14	5.0 0.5
H5	−.0317 45	−.3023 44	.1763 14	4.7 0.6
		(V)		
H2	.2770 33	.6748 96	.8147 48	5.0
H3	.2056 32	.9816 95	.9387 53	5.0
H4	.0958 34	1.2711 89	.7757 50	5.0
H5	.0495 32	1.3416 95	.4799 49	5.0
H8,1	.2244 33	.4322 90	.1203 52	5.0
H8,2	.2748 33	.4603 92	.3123 54	5.0
H10	.3693 30	.3024 92	.0870 48	5.0
H11	.5443 34	.4457 97	.1242 49	5.0
H12	.6335 34	.8028 90	.2654 50	5.0
H13	.5553 33	1.0399 111	.3914 50	5.0
H14	.3884 31	.9465 90	.3599 48	5.0
HM,1	−.0109 37	1.1577 96	.1441 51	5.0
HM,2	.0815 32	1.1345 80	.0888 52	5.0
HM,3	.0671 35	1.3293 97	.2177 51	5.0
		(VI)		
HN2	.9181 18	.5187 36	.4097 20	5.0
H2	.5875 20	.1424 35	.4193 22	5.0
H3	.4706 22	.2128 35	.2247 22	5.0

Table 3. Continued.

Atom	x	y	z	B(Å^2)	Atom	x	y	z	B(Å^2)
H4	.5376	.3774	.1078	5.0	H11	1.2775	.2711	1.0657	5.0
	21	34	23			21	35	24	
H5	.7243	.4860	.1834	5.0	H12	1.3925	.1200	.9941	5.0
	20	36	23			22	34	23	
H8,1	.9499	.1285	.6946	5.0	H13	1.3303	.0305	.7981	5.0
	20	36	22			20	37	22	
H8,2	.9506	.3223	.7573	5.0	H14	1.1483	.0844	.6721	5.0
	20	36	21			20	34	23	
H10	1.0896	.3221	.9363	5.0					
	20	35	21						

methyl derivative (1.408 Å) is significantly longer than that of (VI) (1.375 Å). The reaction rates of these compounds are unknown to the author.

By taking into account the estimated limits of error, it may be seen from Table 6 that none of the bond distances and angles of (I) and (III) differ significantly from the corresponding values for (II) and (VI), respectively. This means that the geometry is unchanged on methylation. By comparing the geometry of (I) with (III), and (II) with (IV) it is also clear that no significant changes occur on substitution of S with O.

The C=N bond of (V) (1.264(5) Å) corresponds to that of α-*p*-dimethylaminobenzaldoxime (1.264(5) Å).[12] The authors point out that this is slightly longer than what, according to Bayer and Hãflinger,[13] is a normal C–N double bond (1.225 Å). However, in cyclohexane-1,4-dioxime [14] the two independent C=N bonds are 1.275(4) Å and 1.277(3) Å, respectively, and the C=N infrared stretching frequency is about 1670 cm^{-1}. The crystal structure determination of diiminosuccinonitrile has recently been carried out,[15] and shows C=N bond distance of 1.275(2) Å. The corresponding IR frequency for this compound is 1630 cm^{-1}. C–N double bond lengths found by microwave investigations of formaldoxime [16] and *N*-methyl-methylenimine [17] are 1.276 Å and 1.30 Å, respectively. The difference between the values above and that of (V) are not significant, and do not account for the high C=N stretching frequencies of iminobenzoxazolines.

The molecules of (VI) form dimers with strong intermolecular hydrogen bonds of length 2.933 Å (Fig. 1 (VI)). Since the hydrogen atom of this bond could not be localized in the difference Fourier map, multiplicity factors of half-hydrogens at N1 and N2 were refined. Five cycles of least squares refinement did not discriminate between the sites. The lowest *R*-factor was obtained with H at a distance of 1.09 Å from N2. However, the *R*-value differences were small, and it cannot be stated with confidence that this is the true position. The N1···H···N2′ distance of (VI) is somewhat shorter than a similar hydrogen bond in isocystine,[18] where two centrosymmetrically related molecules are

Table 4. Observed and calculated structure factors (on 10 times absolute scale).

II

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
1	0	0	299	320	-3	0	1	51	51	2	5	1	34	33	-6	2	2	35	34	-1	8	2	27	28	5	5	3	45	47
2	0	0	45	43	-1	0	1	236	225	3	5	1	52	52	-5	2	2	53	52	0	8	2	31	32	6	5	3	41	37
3	0	0	79	81	0	0	1	44	43	4	5	1	57	56	-4	2	2	97	95	1	8	2	104	104	-6	6	3	24	25
4	0	0	55	57	1	0	1	72	74	5	5	1	85	86	-3	2	2	140	138	2	8	2	68	68	-5	6	3	36	35
5	0	0	93	94	2	0	1	267	283	6	5	1	17	20	-2	2	2	15	18	3	8	2	28	26	-4	6	3	15	20
6	0	0	66	67	3	0	1	180	190	7	5	1	15	17	-1	2	2	120	118	4	8	2	28	27	-2	6	3	37	40
7	0	0	45	44	4	0	1	116	120	-6	6	1	55	55	0	2	2	30	26	5	8	2	58	53	-1	6	3	31	30
8	0	0	91	90	5	0	1	51	57	-5	6	1	62	60	1	2	2	60	54	-4	9	2	37	37	0	6	3	22	24
9	0	0	61	59	8	0	1	42	44	-4	6	1	103	100	2	2	2	172	165	-3	9	2	41	41	1	6	3	18	20
1	1	0	200	209	9	0	1	29	25	-3	6	1	81	80	3	2	2	140	133	-2	9	2	76	76	2	6	3	90	88
2	1	0	137	192	-8	1	1	40	40	-2	6	1	36	35	4	2	2	59	60	-1	9	2	43	41	3	6	3	27	26
3	1	0	126	129	-5	1	1	132	132	-1	6	1	121	118	5	2	2	85	88	0	9	2	40	41	5	6	3	30	29
4	1	0	102	109	-4	1	1	24	25	0	6	1	132	128	6	2	2	68	71	1	9	2	51	50	-5	7	3	20	21
5	1	0	172	180	-3	1	1	58	58	1	6	1	84	81	7	2	2	25	26	-8	0	3	25	25	-4	7	3	37	35
6	1	0	63	63	-2	1	1	375	354	2	6	1	18	19	8	2	2	37	35	-7	0	3	17	15	-3	7	3	57	58
7	1	0	32	32	0	1	1	55	53	3	6	1	171	169	9	2	2	29	26	-5	0	3	112	115	-2	7	3	36	37
8	1	0	44	43	1	1	1	53	50	4	6	1	39	39	-8	3	2	53	53	-4	0	3	220	225	-1	7	3	38	37
9	1	0	65	64	2	1	1	94	84	5	6	1	118	112	-6	3	2	76	76	-3	0	3	13	13	0	7	3	125	121
10	1	0	16	14	3	1	1	155	158	6	6	1	68	70	-5	3	2	40	40	-2	0	3	32	31	1	7	3	13	16
0	2	0	476	477	4	1	1	220	229	7	6	1	24	24	-4	3	2	32	32	-1	0	3	57	57	2	7	3	45	44
1	2	0	210	210	5	1	1	62	64	8	6	1	30	33	-3	3	2	38	38	0	0	3	42	40	3	7	3	47	45
2	2	0	14	16	6	1	1	31	30	-6	7	1	83	82	-2	3	2	118	116	1	0	3	114	116	4	7	3	31	29
3	2	0	224	233	7	1	1	153	154	-5	7	1	27	27	-1	3	2	49	46	2	0	3	68	70	5	7	3	22	18
4	2	0	80	83	8	1	1	55	54	-4	7	1	49	48	0	3	2	154	149	4	0	3	173	183	-3	8	3	34	34
5	2	0	172	175	9	1	1	26	24	-3	7	1	78	78	1	3	2	68	67	5	0	3	63	66	-1	8	3	21	22
6	2	0	96	97	10	1	1	26	22	-2	7	1	117	119	2	3	2	172	162	6	0	3	27	28	0	8	3	14	13
7	2	0	57	55	-9	2	1	28	26	-1	7	1	56	55	3	3	2	143	140	7	0	3	20	21	1	8	3	19	21
8	2	0	21	22	-8	2	1	14	15	0	7	1	19	18	4	3	2	132	130	8	0	3	38	36	2	8	3	36	36
9	2	0	44	43	-7	2	1	106	106	1	7	1	70	67	5	3	2	75	75	-6	1	3	25	28	-6	0	4	75	78
1	3	0	340	344	-6	2	1	70	68	2	7	1	90	92	6	3	2	19	19	-5	1	3	61	64	-5	0	4	26	27
2	3	0	190	200	-5	2	1	72	71	3	7	1	54	55	7	3	2	45	46	-4	1	3	57	60	-3	0	4	25	25
3	3	0	60	59	-4	2	1	60	63	5	7	1	42	43	9	3	2	31	26	-3	1	3	18	18	-2	0	4	47	49
4	3	0	77	77	-3	2	1	106	106	6	7	1	24	21	-7	4	2	26	25	-2	1	3	29	29	1	0	4	49	49
5	3	0	43	45	-2	2	1	128	120	7	7	1	27	25	-6	4	2	28	28	-1	1	3	90	91	2	0	4	30	29
6	3	0	29	28	-1	2	1	237	223	-6	8	1	55	54	-5	4	2	69	65	0	1	3	68	68	3	0	4	14	12
7	3	0	71	73	0	2	1	234	228	-5	8	1	59	57	-4	4	2	141	139	1	1	3	101	102	5	0	4	22	22
8	3	0	55	54	1	2	1	35	34	-4	8	1	38	38	-3	4	2	29	30	2	1	3	18	19	6	0	4	29	27
0	4	0	106	103	2	2	1	193	187	-1	8	1	98	99	-2	4	2	170	170	3	1	3	41	47	-6	1	4	52	56
1	4	0	58	59	3	2	1	64	61	0	8	1	101	100	-1	4	2	161	157	4	1	3	47	50	-5	1	4	43	49
2	4	0	70	73	4	2	1	28	27	2	8	1	77	77	0	4	2	150	142	5	1	3	55	61	-4	1	4	27	28
3	4	0	141	143	5	2	1	69	72	3	8	1	121	126	1	4	2	26	23	6	1	3	44	42	-2	1	4	12	13
4	4	0	52	52	6	2	1	86	89	4	8	1	22	24	2	4	2	71	70	-8	2	3	24	23	-1	1	4	80	81
5	4	0	93	94	7	2	1	32	33	5	8	1	25	26	3	4	2	44	41	-6	2	3	26	24	0	1	4	76	75
6	4	0	128	130	9	2	1	31	29	6	8	1	42	39	4	4	2	47	47	-5	2	3	94	96	2	1	4	51	55
7	4	0	75	80	-9	3	1	48	43	-5	9	1	36	34	5	4	2	60	60	-4	2	3	104	105	3	1	4	106	110
8	4	0	42	40	-8	3	1	63	59	-3	9	1	74	75	6	4	2	26	26	-3	2	3	36	36	5	1	4	33	34
1	5	0	238	241	-7	3	1	60	58	-2	9	1	88	90	7	4	2	36	36	-2	2	3	45	45	6	1	4	25	24
2	5	0	183	189	-6	3	1	45	45	-1	9	1	37	35	8	4	2	43	39	-1	2	3	116	114	-6	2	4	41	44
3	5	0	113	114	-5	3	1	78	77	0	9	1	43	43	-7	5	2	35	34	0	2	3	49	50	-5	2	4	47	49
4	5	0	81	86	-4	3	1	55	53	1	9	1	34	34	-6	5	2	25	24	1	2	3	168	162	-4	2	4	17	21
5	5	0	29	30	-3	3	1	151	157	2	9	1	23	23	-5	5	2	56	54	2	2	3	74	72	-3	2	4	33	33
6	5	0	48	51	-2	3	1	181	178	3	9	1	34	37	-4	5	2	13	14	3	2	3	19	17	-2	2	4	38	39
7	5	0	52	55	-1	3	1	70	70	4	9	1	53	53	-3	5	2	20	22	4	2	3	67	67	-1	2	4	31	32
8	5	0	45	46	0	3	1	107	108	-3	10	1	28	25	-2	5	2	90	92	5	2	3	39	40	0	2	4	24	25
0	6	0	66	69	1	3	1	190	184	-1	10	1	53	53	-1	5	2	16	13	7	2	3	44	38	1	2	4	58	58
1	6	0	76	78	2	3	1	242	228	0	10	1	55	56	0	5	2	23	22	8	2	3	38	35	2	2	4	34	34
2	6	0	55	58	3	3	1	54	55	2	10	1	40	41	1	5	2	16	18	-7	3	3	23	20	3	2	4	20	20
3	6	0	53	54	4	3	1	221	220	3	10	1	22	23	3	5	2	158	152	-6	3	3	43	43	-4	3	4	30	30
4	6	0	33	35	5	3	1	70	72	-8	0	2	36	34	4	5	2	141	137	-5	3	3	42	43	-3	3	4	37	39
5	6	0	40	42	7	3	1	18	18	-7	0	2	34	34	5	5	2	70	71	-4	3	3	64	65	-2	3	4	24	25
6	6	0	84	85	8	3	1	18	23	-6	0	2	52	53	7	5	2	41	45	-3	3	3	100	103	-1	3	4	53	53
7	6	0	54	56	-9	4	1	16	15	-5	0	2	51	50	-7	6	2	64	61	-2	3	3	39	39	0	3	4	70	68
1	7	0	87	90	-8	4	1	20	23	-4	0	2	31	29	-6	6	2	25	26	0	3	3	28	30	2	3	4	35	35
2	7	0	75	76	-7	4	1	47	45	-3	0	2	145	142	-5	6	2	59	57	1	3	3	28	28	5	3	4	30	28
3	7	0	21	23	-6	4	1	37	35	-2	0	2	244	238	-4	6	2	86	85	2	3	3	49	48	-5	4	4	37	37
4	7	0	154	163	-5	4	1	62	61	-1	0	2	129	128	-3	6	2	26	28	3	3	3	121	115	-4	4	4	27	31
5	7	0	64	67	-4	4	1	148	143	0	0	2	56	65	-2	6	2	74	75	4	3	3	55	54	-2	4	4	17	14
6	7	0	24	26	-3	4	1	152	153	1	0	2	138	142	-1	6	2	109	107	5	3	3	40	38	-1	4	4	23	24
7	7	0	34	34	-2	4	1	169	164	2	0	2	251	261	0	6	2	81	78	6	3	3	48	45	0	4	4	63	62
0	8	0	109	109	-1	4	1	153	150	3	0	2	113	118	1	6	2	140	139	7	3	3	21	21	1	4	4	87	79
1	8	0	112	119	0	4	1	258	247	5	0	2	78	82	2	6	2	65	64	-6	4	3	23	23	2	4	4	71	68
2	8	0	49	52	1	4	1	71	68	6	0	2	172	182	3	6	2	37	37	-5	4	3	34	34	4	4	4	47	48
3	8	0	41	44	2	4	1	31	30	8	0	2	42	39	5	6	2	54	52	-2	4	3	68	69	-4	5	4	31	30
5	8	0	16	20	3	4	1	41	42	-9	1	2	35	32	6	6	2	14	11	-1	4	3	64	63	-3	5	4	38	40
6	8	0	26	27	4	4	1	89	88	-8	1	2	69	66	-6	7	2	39	38	0	4	3	35	33	-2	5	4	28	29
1	9	0	69	72	5	4	1	135	138	-7	1	2	23	22	-5	7	2	35	33	1	4	3	109	106	-1	5	4	41	43
2	9	0	21	21	6	4	1	129	127	-6	1	2	45	46	-4	7	2	38	36	2	4	3	107	105	0	5	4	21	20
3	9	0	40	42	7	4	1	37	38	-5	1	2	26	28	-3	7	2	59	58	3	4	3	55	52	1	5	4	15	17
4	9	0	57	61	8	4	1	47	49	-4	1	2	103	102	-2	7	2	93	94	4	4	3	29	28	-3	6	4	19	18
5	9	0	54	57	9	4	1	30	28	-3	1	2	402	393	-1	7	2	31	31	5	4	3	19	17	-2	6	4	25	25
0	10	0	57	55	-8	5	1	74	70	-2	1	2	161	159	0	7	2	21	20	7	4	3	43	38	-1	6	4	47	46
1	10	0	50	54	-7	5	1	58	56	-1	1	2	23	21	1	7	2	49	49	-6	5	3	44	44	0	6	4	52	51
2	10	0	17	18	-6	5	1	50	49	0	1	2	129	126	2	7	2	87	87	-5	5	3	43	45	1	6	4	61	60
3	10	0	36	37	-5	5	1	56	53	1	1	2	148	143	3	7	2	70	69	-4	5	3	49	49	2	6	4	35	35
10	0	1	67	63	-4	5	1	23	23	2	1	2	72	68	4	7	2	57	56	-3	5	3	90	92	-2	0	5	38	39
-8	0	1	22	21	-3	5	1	94	92	3	1	2	56	57	6	7	2	28	27	-2	5	3	70	69	1	0	5	34	37
-7	0	1	105	108	-2	5	1	96	95	4	1	2	78	84	-5	8	2	23	24	-1	5	3	30	29	2	0	5	46	51
-6	0	1	112	113	-1	5	1	90	84	5	1	2	74	74	-4	8	2	67	65	0	5	3	81	79	-2	1	5	35	37
-5	0	1	32	34	0	5	1	106	105	6	1	2	67	66	-3	8	2	29	31	1	5	3	40	41	-1	1	5	25	27
-4	0	1	18	18	1	5	1	200	198	9	1	2	41	36	-2	8	2	31	31	2	5	3	85	84	1	1	5	43	43
																				3	5	3	86	84	2	1	5	21	20
																				4	5	3	36	36	0	2	5	28	29
																									1	2	5	35	39

III

h	k	l	Fo	Fc	h	k	l	Fo	Fc	k	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
					0	0	22	32	32	1	0	-12	208	207	2	0	-28	45	47	2	0	14	147	-150	3	0	-6	175	169
0	0	3	7	0	0	0	23	12	0	1	0	-8	493	491	2	0	-26	47	49	2	0	16	26	-28	3	0	-4	204	208
0	0	4	787	-786	0	0	24	109	105	1	0	-4	313	320	2	0	-24	12	11	2	0	18	181	180	3	0	-2	162	165
0	0	5	8	0	0	0	25	13	0	1	0	-2	483	-473	2	0	-22	30	32	2	0	20	145	-146	3	0	0	39	-36
0	0	6	52	-51	0	0	26	12	7	1	0	0	801	-802	2	0	-20	33	-31	2	0	22	73	-76	3	0	2	248	-239
0	0	7	8	0	0	0	27	12	0	1	0	2	492	480	2	0	-18	165	-165	2	0	24	70	72	3	0	4	93	93
0	0	8	236	-235	0	0	28	29	-28	1	0	4	120	119	2	0	-16	10	-11	2	0	26	12	9	3	0	6	124	118
0	0	9	10	0	0	0	30	12	-6	1	0	6	156	150	2	0	-14	143	147	3	0	-32	19	-16	3	0	8	51	-48
0	0	10	58	-56	0	0	32	13	8	1	0	8	152	-155	2	0	-12	141	141	3	0	-30	33	-33	3	0	10	116	114
0	0	11	11	0	1	0	-34	24	-25	1	0	10	294	-287	2	0	-10	173	168	3	0	-28	46	45	3	0	12	72	73
0	0	12	296	-292	1	0	-32	37	37	1	0	12	325	-324	2	0	-8	106	-111	3	0	-26	39	-37	3	0	14	30	-34
0	0	13	13	0	1	0	-30	95	94	1	0	14	100	-97	2	0	-6	9	-4	3	0	-24	22	-22	3	0	16	17	-114
0	0	14	202	200	1	0	-28	14	15	1	0	16	217	217	2	0	-4	68	69	3	0	-22	112	111	3	0	20	42	44
0	0	15	12	0	1	0	-26	68	-67	1	0	18	11	7	2	0	-2	411	-412	3	0	-20	104	105	4	0	-32	68	66
0	0	16	151	150	1	0	-24	76	-76	1	0	20	114	112	2	0	0	555	-551	3	0	-18	88	86	4	0	-28	98	-100
0	0	17	13	0	1	0	-22	102	-97	1	0	22	111	111	2	0	2	187	179	3	0	-16	182	-185	4	0	-26	73	73
0	0	18	192	-188	1	0	-20	17	13	1	0	24	87	-88	2	0	6	315	-306	3	0	-14	66	-70	4	0	-24	18	18
0	0	19	13	0	1	0	-18	101	102	1	0	28	12	-11	2	0	8	291	297	3	0	-12	39	38	4	0	-22	69	-69
0	0	20	85	-84	1	0	-16	212	-210	2	0	-32	75	-71	2	0	10	285	282	3	0	-10	345	-356	4	0	-20	12	-9
0	0	21	11	0	1	0	-14	85	84	2	0	-30	50	-48	2	0	12	115	117	3	0	-8	73	-75	4	0	-18	34	34

Table 4. Continued.

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
4	0	-16	50	52	1	1	19	21	-22	4	1	-25	75	74	0	2	29	45	41	3	2	-13	56	59	0	3	16	33	29
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1	1	6	16	-12	3	1	22	20	19	0	2	19	44	-46	3	2	-23	25	27	0	3	6	35	35	3	3	-11	49	-51
1	1	7	9	3	3	1	24	17	-14	0	2	20	40	40	3	2	-22	13	15	0	3	7	17	16	3	3	-10	181	-183
1	1	8	133	-136	3	1	25	13	-5	0	2	21	107	-111	3	2	-21	33	-36	0	3	8	13	13	3	3	-9	34	33
1	1	10	307	301	4	1	-32	25	25	0	2	22	67	-72	3	2	-20	88	84	0	3	9	24	-28	3	3	-8	62	-59
1	1	11	24	26	4	1	-31	13	-8	0	2	23	20	-25	3	2	-19	59	-59	0	3	10	30	31	3	3	-7	28	21
1	1	12	66	-69	4	1	-30	19	-16	0	2	24	67	-64	3	2	-18	18	20	0	3	11	102	-103	3	3	-6	25	27
1	1	14	244	-239	4	1	-29	24	-24	0	2	25	28	33	3	2	-17	77	75	0	3	12	42	45	3	3	-5	54	-53
1	1	16	113	-116	4	1	-28	24	21	0	2	26	59	59	3	2	-16	12	5	0	3	13	12	-4	3	3	-4	74	77
1	1	17	42	41	4	1	-27	20	18	0	2	27	35	-32	3	2	-15	25	26	0	3	14	[illegible]	[illegible]	3	3	-3	47	-46
1	1	18	60	60	4	1	-26	18	16	0	2	28	13	10	3	2	-14	38	-43	0	3	15	55	-54	3	3	-2	12	7

Table 4. Continued.

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
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3	3	0	48	-47	4	3	-1	47	-44	0	4	6	12	-2	1	4	-2	39	-38	2	4	2	40	-38	3	4	7	29	-31
3	3	1	58	59	4	3	0	39	37	0	4	7	16	9	1	4	-1	22	21	2	4	3	13	6	3	4	8	13	-10
3	3	2	64	65	4	3	1	24	26	0	4	8	90	87	1	4	0	28	26	2	4	4	67	66	3	4	9	36	38
3	3	3	98	-98	4	3	2	32	27	0	4	9	45	-45	1	4	1	48	47	2	4	5	21	-21	3	4	11	23	24
3	3	4	26	-25	4	3	3	27	25	0	4	10	36	-37	1	4	2	42	41	2	4	6	13	-5	4	4	-12	13	9
3	3	5	36	38	4	3	4	15	16	0	4	11	35	-37	1	4	3	35	-37	2	4	7	55	54	4	4	-9	13	9
3	3	6	91	-95	4	3	5	65	-67	0	4	12	13	-3	1	4	4	32	31	2	4	8	25	-26	4	4	-7	13	4
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3	3	8	40	42	4	3	7	56	56	0	4	14	34	33	1	4	7	18	-12	2	4	10	61	57	4	4	-3	23	21
3	3	9	64	-65	4	3	8	13	12	0	4	15	28	26	1	4	8	12	-3	2	4	11	55	-52	4	4	-2	17	-17
3	3	10	83	79	4	3	9	36	37	0	4	16	15	-15	1	4	9	13	-2	2	4	12	44	-41	4	4	-1	21	-19
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4	3	-4	54	-58	0	4	4	71	-71	1	4	-4	21	-21	2	4	0	57	-58	3	4	4	53	-54					

IV

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
0	0	2	199	204	0	4	8	74	76	1	1	16	82	85	1	5	12	25	26	2	2	17	67	67	3	0	4	121	118
0	0	4	653	738	0	4	9	13	8	1	1	17	75	76	1	5	13	81	79	2	2	18	27	28	3	0	5	19	18
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0	0	8	258	267	0	4	11	38	42	1	1	19	48	49	1	5	15	41	40	2	2	20	14	18	3	0	7	28	29
0	0	10	105	107	0	4	12	111	112	1	1	21	41	41	1	5	16	28	29	2	2	21	36	33	3	0	8	14	15
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0	4	1	178	186	1	1	9	70	70	1	5	5	15	15	2	2	9	169	171	2	7	2	37	37	3	4	6	47	46
0	4	2	35	36	1	1	10	190	196	1	5	6	73	77	2	2	10	22	21	2	7	3	24	25	3	4	7	74	73
0	4	3	51	51	1	1	11	99	98	1	5	7	93	97	2	2	12	59	60	2	7	4	29	26	3	4	8	40	38
0	4	4	92	99	1	1	12	72	73	1	5	8	49	48	2	2	13	102	105	2	7	5	38	34	3	4	9	21	24
0	4	5	154	159	1	1	13	42	43	1	5	9	99	101	2	2	14	69	71	2	7	6	12	11	3	4	10	24	21
0	4	6	114	119	1	1	14	34	33	1	5	10	62	63	2	2	15	34	36	2	7	7	17	17	3	4	11	31	31
0	4	7	48	48	1	1	15	54	54	1	5	11	34	32	2	2	16	52	54	3	0	2	32	32	3	4	12	63	61
																				3	0	3	64	64					

Table 4. Continued.

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
3	4	13	18	15	3	6	2	20	19	4	1	5	47	48	4	2	9	17	16	4	3	12	36	34	5	0	6	53	50
3	4	14	30	20	3	6	4	32	31	4	1	6	35	38	4	2	11	36	37	4	3	13	42	41	5	0	7	31	29
3	4	15	24	24	3	6	7	22	21	4	1	7	38	36	4	2	12	37	40	4	4	0	30	31	5	0	8	23	25
3	4	16	21	20	3	6	8	24	22	4	1	8	65	64	4	2	13	30	41	4	4	2	23	22	5	1	0	44	43
3	5	0	26	26	4	0	1	21	22	4	1	9	15	17	4	2	14	37	37	4	4	3	47	46	5	1	1	15	15
3	5	1	42	44	4	0	2	32	33	4	1	10	38	39	4	2	15	37	37	4	4	5	42	41	5	1	2	29	30
3	5	2	29	30	4	0	5	59	57	4	1	11	14	16	4	3	0	10	17	4	4	6	50	48	5	1	3	20	20
3	5	3	11	13	4	0	7	11	15	4	1	12	39	38	4	3	1	78	69	4	4	7	45	42	5	1	4	49	49
3	5	4	42	40	4	0	8	51	51	4	1	13	23	25	4	3	2	59	60	4	4	8	13	9	5	1	5	12	9
3	5	5	46	45	4	0	9	68	69	4	1	15	21	23	4	3	3	32	33	4	4	9	41	40	5	1	6	20	31
3	5	6	26	26	4	0	10	83	83	4	2	0	19	21	4	3	4	55	51	4	4	10	25	22	5	1	7	14	11
3	5	7	33	32	4	0	11	17	16	4	2	1	56	57	4	3	5	52	52	4	5	0	18	12	5	1	8	18	17
3	5	8	29	27	4	0	13	21	25	4	2	2	59	61	4	3	6	48	49	4	5	1	18	15	5	2	0	61	62
3	5	9	18	17	4	0	14	23	26	4	2	3	71	72	4	3	7	44	44	4	5	3	11	10	5	2	1	18	21
3	5	10	41	42	4	1	0	71	70	4	2	4	38	38	4	3	8	24	22	5	0	1	25	23	5	2	2	72	71
3	5	11	31	30	4	1	1	35	36	4	2	5	50	50	4	3	9	15	17	5	0	3	22	20	5	2	3	24	22
3	5	12	17	15	4	1	2	51	53	4	2	6	53	54	4	3	10	35	37	5	0	4	19	22	5	2	4	27	20
3	5	13	17	18	4	1	3	12	10	4	2	7	55	55	4	3	11	38	30	5	0	5	26	25	5	2	5	13	14
3	6	0	30	32	4	1	4	11	12	4	2	8	15	17															

V

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
0	0	-8	53	54	6	0	3	90	88	0	1	2	410	395	6	1	-1	180	176	13	1	1	32	33	5	2	-7	45	49
0	0	-6	120	120	6	0	4	26	24	0	1	3	178	175	6	1	0	304	290	14	1	-9	42	37	5	2	-5	69	69
0	0	-5	29	34	6	0	5	22	21	0	1	4	273	265	6	1	1	149	110	14	1	-8	52	50	5	2	-4	110	108
0	0	-4	176	174	7	0	-8	47	51	0	1	5	92	89	6	1	2	35	35	14	1	-7	17	16	5	2	-2	173	179
0	0	-3	302	302	7	0	-5	90	90	0	1	6	69	67	6	1	3	45	47	14	1	-6	32	29	5	2	-1	142	140
0	0	-2	589	623	7	0	-4	35	34	0	1	7	75	75	6	1	4	73	76	14	1	-5	45	46	5	2	0	226	223
0	0	-1	344	335	7	0	-3	131	133	0	1	8	51	49	6	1	5	62	62	14	1	-4	23	21	5	2	1	36	33
0	0	1	344	335	7	0	-2	57	59	1	1	-9	21	20	6	1	6	20	23	14	1	-2	18	16	5	2	2	21	26
0	0	2	597	623	7	0	-1	90	88	1	1	-8	25	20	7	1	-9	20	17	14	1	-1	23	27	5	2	3	20	20
0	0	3	308	302	7	0	0	90	94	1	1	-7	40	38	7	1	-8	115	115	14	1	0	35	35	5	2	4	21	24
0	0	4	176	174	7	0	1	51	50	1	1	-6	59	60	7	1	-7	114	118	15	1	-8	39	40	5	2	6	40	34
0	0	5	30	34	7	0	3	91	93	1	1	-4	124	120	7	1	-6	32	31	15	1	-7	36	37	6	2	-8	70	69
0	0	6	122	120	7	0	4	17	16	1	1	-3	211	214	7	1	-5	78	79	15	1	-6	46	44	6	2	-7	94	94
0	0	8	55	54	7	0	5	65	66	1	1	-2	210	212	7	1	-4	137	133	15	1	-5	27	22	6	2	-6	30	28
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1	0	-8	97	99	8	0	-8	107	107	1	1	0	445	431	7	1	-2	15	9	15	1	-3	26	24	6	2	-4	149	154
1	0	-7	103	107	8	0	-7	29	35	1	1	1	335	330	7	1	-1	81	82	15	1	-2	27	27	6	2	-3	30	31
1	0	-6	20	19	8	0	-6	42	46	1	1	2	224	221	7	1	0	70	66	15	1	-1	18	16	6	2	-2	58	57
1	0	-5	101	100	8	0	-5	135	135	1	1	3	60	56	7	1	1	120	120	0	2	-8	21	27	6	2	-1	277	280
1	0	-4	72	70	8	0	-4	113	110	1	1	4	84	85	7	1	2	68	73	0	2	-7	36	37	6	2	0	110	114
1	0	-3	165	166	8	0	-3	20	18	1	1	5	101	101	7	1	3	66	68	0	2	-6	59	64	6	2	1	62	60
1	0	-2	305	303	8	0	-1	89	87	1	1	6	33	35	7	1	5	62	65	0	2	-5	38	47	6	2	2	45	42
1	0	-1	17	19	8	0	0	18	13	1	1	7	54	52	8	1	-10	21	17	0	2	-4	159	157	6	2	3	55	53
1	0	0	59	57	8	0	1	172	181	1	1	8	22	26	8	1	-9	23	22	0	2	-3	202	209	6	2	5	46	44
1	0	1	380	386	8	0	2	52	53	2	1	-9	19	16	8	1	-8	60	60	0	2	-2	28	28	7	2	-9	40	40
1	0	2	156	157	8	0	4	59	62	2	1	-8	31	30	8	1	-7	83	85	0	2	-1	146	158	7	2	-8	52	53
1	0	3	54	55	8	0	5	23	27	2	1	-7	62	59	8	1	-6	65	60	0	2	0	97	99	7	2	-7	100	102
1	0	4	33	32	9	0	-9	18	14	2	1	-6	45	47	8	1	-5	54	56	0	2	1	169	158	7	2	-6	73	75
1	0	5	61	63	9	0	-6	60	60	2	1	-5	63	63	8	1	-4	16	17	0	2	2	28	28	7	2	-5	33	39
1	0	7	86	85	9	0	-5	23	23	2	1	-4	141	137	8	1	-3	31	31	0	2	3	212	209	7	2	-4	92	100
1	0	8	37	45	9	0	-3	127	123	2	1	-3	72	73	8	1	-2	102	100	0	2	4	161	157	7	2	-3	116	112
2	0	-8	37	44	9	0	-1	157	154	2	1	-2	168	172	8	1	-1	44	45	0	2	5	53	47	7	2	-2	34	38
2	0	-7	128	123	9	0	0	53	53	2	1	-1	268	285	8	1	0	46	42	0	2	6	62	64	7	2	-1	273	271
2	0	-6	27	30	9	0	1	54	56	2	1	0	549	556	8	1	1	55	58	0	2	7	34	37	7	2	0	120	120
2	0	-5	135	135	9	0	2	58	61	2	1	1	135	129	8	1	2	16	13	0	2	8	21	27	7	2	1	88	87
2	0	-4	65	67	9	0	4	75	80	2	1	2	222	215	8	1	3	93	93	1	2	-9	25	26	7	2	2	54	55
2	0	-3	138	131	10	0	-8	94	97	2	1	3	89	89	8	1	4	64	65	1	2	-8	34	35	7	2	3	81	81
2	0	-2	119	118	10	0	-7	197	208	2	1	4	51	47	8	1	5	31	34	1	2	-7	67	69	8	2	-9	43	41
2	0	-1	81	83	10	0	-6	60	61	2	1	5	49	48	9	1	-10	21	24	1	2	-6	92	93	8	2	-8	51	49
2	0	0	169	165	10	0	-5	52	54	2	1	6	61	58	9	1	-9	21	19	1	2	-5	23	24	8	2	-6	58	56
2	0	1	193	186	10	0	-4	94	92	2	1	7	51	45	9	1	-8	77	79	1	2	-4	180	178	8	2	-5	35	36
2	0	2	18	17	10	0	-3	130	136	2	1	8	22	25	9	1	-7	57	59	1	2	-3	111	108	8	2	-4	38	36
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2	0	5	37	32	10	0	0	45	45	3	1	-6	33	29	9	1	-4	106	106	1	2	0	188	196	8	2	-1	111	107
2	0	6	32	36	10	0	2	19	17	3	1	-5	97	93	9	1	-3	95	91	1	2	1	185	167	8	2	0	154	153
2	0	8	18	16	10	0	3	43	48	3	1	-4	282	271	9	1	-2	62	60	1	2	2	113	97	8	2	1	39	37
3	0	-8	93	96	10	0	4	26	29	3	1	-3	174	169	9	1	-1	27	26	1	2	3	163	159	8	2	2	101	103
3	0	-7	15	11	11	0	-10	19	19	3	1	-2	250	252	9	1	0	54	51	1	2	4	93	80	8	2	4	38	40
3	0	-6	94	95	11	0	-9	77	79	3	1	-1	386	400	9	1	1	27	23	1	2	5	156	150	9	2	-9	22	20
3	0	-5	64	64	11	0	-8	97	97	3	1	0	580	584	9	1	2	50	51	1	2	6	25	23	9	2	-8	78	79
3	0	-4	27	28	11	0	-7	49	52	3	1	1	97	93	9	1	3	38	37	1	2	7	38	39	9	2	-7	62	63
3	0	-3	35	34	11	0	-6	41	43	3	1	2	157	148	10	1	-9	36	37	2	2	-7	60	62	9	2	-6	61	64
3	0	-2	241	243	11	0	-5	138	138	3	1	3	193	188	10	1	-8	58	55	2	2	-6	48	46	9	2	-4	51	66
3	0	-1	343	345	11	0	-4	20	15	3	1	4	133	128	10	1	-7	60	64	2	2	-5	26	17	9	2	-1	83	81
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3	0	1	132	133	11	0	-2	43	44	3	1	6	41	40	10	1	-5	81	80	2	2	-3	55	56	9	2	1	94	93
3	0	2	27	31	11	0	0	24	28	3	1	7	55	55	10	1	-4	16	17	2	2	-2	134	152	9	2	2	47	46
3	0	4	35	36	11	0	1	50	54	3	1	8	23	25	10	1	-3	138	138	2	2	-1	108	118	9	2	3	69	71
3	0	5	111	115	11	0	2	22	25	4	1	-10	18	20	10	1	-2	59	58	2	2	0	124	125	9	2	4	36	38
3	0	6	70	75	11	0	3	31	33	4	1	-9	19	14	10	1	-1	80	78	2	2	1	68	69	10	2	-9	42	41
4	0	-8	50	52	12	0	-10	24	25	4	1	-8	93	94	10	1	0	52	50	2	2	2	226	211	10	2	-8	50	49
4	0	-7	108	113	12	0	-9	30	32	4	1	-7	92	95	10	1	1	56	57	2	2	3	150	153	10	2	-7	39	42
4	0	-6	85	87	12	0	-8	31	29	4	1	-6	68	70	10	1	2	59	58	2	2	4	64	65	10	2	-6	35	32
4	0	-5	143	149	12	0	-7	19	16	4	1	-5	76	69	10	1	3	21	19	2	2	5	90	89	10	2	-5	56	57
4	0	-4	104	109	12	0	-6	77	78	4	1	-4	62	60	10	1	4	55	53	2	2	6	71	69	10	2	-3	84	81
4	0	-3	220	222	12	0	-5	48	46	4	1	-3	27	24	11	1	-10	24	26	2	2	8	29	28	10	2	-1	130	132
4	0	-2	131	131	12	0	-4	41	39	4	1	-2	45	48	11	1	-9	31	27	3	2	-9	33	34	10	2	0	64	64
4	0	-1	184	188	12	0	-3	93	95	4	1	-1	329	325	11	1	-8	61	62	3	2	-8	41	40	10	2	1	61	60
4	0	2	23	25	12	0	-1	62	64	4	1	0	384	377	11	1	-7	44	41	3	2	-7	63	62	10	2	2	27	31
4	0	3	54	57	12	0	0	28	30	4	1	1	60	59	11	1	-6	71	70	3	2	-6	132	131	10	2	3	26	19
4	0	4	36	34	13	0	-8	120	120	4	1	2	91	87	11	1	-5	79	77	3	2	-5	43	46	11	2	-9	23	20
4	0	5	16	16	13	0	-7	100	100	4	1	3	125	124	11	1	-4	47	45	3	2	-3	93	93	11	2	-8	24	24
4	0	6	37	35	13	0	-6	44	41	4	1	4	21	25	11	1	-3	40	38	3	2	-2	74	79	11	2	-6	91	91
4	0	7	25	29	13	0	-5	18	13	4	1	5	55	55	11	1	-2	48	47	3	2	-1	97	101	11	2	-5	41	43
5	0	-9	25	26	13	0	-4	72	72	4	1	6	32	31	11	1	-1	52	52	3	2	0	140	140	11	2	-4	89	92
5	0	-8	23	25	13	0	-3	30	29	4	1	7	27	28	11	1	0	47	45	3	2	1	146	130	11	2	-3	38	37
5	0	-7	30	32	13	0	-2	73	74	5	1	-8	72	74	11	1	1	68	69	3	2	2	148	144	11	2	-2	99	98
5	0	-6	16	15	13	0	-1	33	32	5	1	-7	80	80	11	1	3	42	39	3	2	3	33	33	11	2	-1	33	31
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5	0	-2	36	35	14	0	-7	33	32	5	1	-3	124	120	12	1	-6	89	89	4	2	-9	33	32	12	2	-6	38	36
5	0	-1	27	32	14	0	-6	17	17	5	1	-2	58	58	12	1	-5	88	82	4	2	-8	60	58	12	2	-5	99	99
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5	0	1	104	101	14	0	-1	38	40	5	1	0	160	158	12	1	-3	60	59	4	2	-6	73	74	12	2	-3	31	30
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5	0	3	96	97	15	0	-6	24	23	5	1	2	115	115	12	1	-1	18	17	4	2	-4	88	89	12	2	-1	56	54
5	0	4	63	63	15	0	-5	37	34	5	1	3	66	66	12	1	0	18	22	4	2	-3	160	155	12	2	0	26	28
5	0	5	56	58	15	0	-4	32	34	5	1	4	58	58	12	1	1	37	36	4	2	-2	164	179	12	2	1	35	42
6	0	-8	55	57	15	0	-1	37	32	5	1	5	78	77	12	1	2	47	45	4	2	-1	241	249	13	2	-8	24	27
6	0	-6	61	64	0	1	-8	50	49	5	1	6	32	33	13	1	-9	46	43	4	2	0	138	134	13	2	-6	28	26
6	0	-5	66	65	0	1	-7	73	75	5	1	7	24	28	13	1	-8	38	34	4	2	1	43	38	13	2	-4	41	42
6	0	-4	202	204	0	1	-6	68	67	6	1	-9	36	39	13	1	-6	54	56	4	2	2	62	61	13	2	-3	57	56
6	0	-3	16	20	0	1	-5	91	89	6	1	-7	26	25	13	1	-5	49	49	4	2	3	26	24	13	2	-2	21	18
6	0	-2	118	117	0	1	-4	261	265	6	1	-6	97	97	13	1	-4	73	72	4	2	4	69	69	13	2	-1	49	50
6	0	-1	232	227	0	1	-3	168	175	6	1	-5	122	114	13	1	-3	60	60	4	2	6	48	45	14	2	-7	32	29
6	0	0	147	150	0	1	-2	389	395	6	1	-4	160	155	13	1	-2	47	44	4	2	7	31	25	14	2	-6	50	51
6	0	1	64	66	0	1	-1	407	439	6	1	-3	54	54	13	1	-1	64	63	5	2	-9	18	21	14	2	-5	22	12
6	0	2	67	69	0	1	1	460	439	6	1	-2	202	194	13	1	0	30	30	5	2	-8	56	54	14	2	-4	35	37

Table 4. Continued.

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
14	2	-3	46	48	3	3	5	31	32	9	3	-9	27	25	1	4	-2	23	27	6	4	-3	19	42	1	5	5	28	28
14	2	-2	43	43	4	3	-8	26	24	9	3	-7	24	22	1	4	-1	18	38	6	4	-2	65	69	2	5	-6	18	15
15	2	-5	36	38	4	3	-7	81	75	9	3	-6	73	75	1	4	0	20	29	6	4	-1	70	71	2	5	-5	46	45
15	2	-4	40	40	4	3	-6	56	54	9	3	-5	88	87	1	4	1	85	79	6	4	0	36	48	2	5	-3	21	19
15	2	-2	38	42	4	3	-5	43	46	9	3	-4	30	31	1	4	2	33	32	6	4	1	60	69	2	5	-2	79	69
0	3	-8	25	23	4	3	-3	78	78	9	3	-3	24	26	1	4	3	38	37	6	4	3	43	40	2	5	-1	40	50
0	3	-7	60	58	4	3	-2	64	68	9	3	-2	64	63	1	4	4	40	42	7	4	-8	21	13	2	5	0	41	47
0	3	-6	48	50	4	3	-1	104	101	9	3	1	31	36	1	4	5	20	18	7	4	-7	24	25	2	5	1	35	36
0	3	-5	143	144	4	3	0	84	79	9	3	2	19	20	1	4	6	22	21	7	4	-6	37	37	2	5	2	39	34
0	3	-4	43	46	4	3	1	103	109	10	3	-9	43	41	2	4	-7	22	22	7	4	-5	47	47	2	5	3	24	22
0	3	-3	70	71	4	3	2	36	38	10	3	-7	34	36	2	4	-6	42	37	7	4	-4	40	43	2	5	4	21	20
0	3	-2	150	155	4	3	3	103	100	10	3	-6	47	47	2	4	-5	63	64	7	4	-2	41	49	3	5	-5	34	35
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0	3	1	72	68	4	3	5	23	18	10	3	-3	39	42	2	4	-2	55	56	7	4	0	53	51	3	5	-3	38	36
0	3	2	171	159	4	3	6	21	23	10	3	-2	94	92	2	4	-1	65	64	7	4	1	42	33	3	5	-2	27	26
0	3	3	72	71	5	3	-9	25	23	10	3	-1	60	58	2	4	0	53	61	7	4	2	33	30	3	5	-1	59	66
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1	3	-7	84	83	5	3	-1	95	96	11	3	-5	17	18	2	4	6	46	42	8	4	-1	68	71	4	5	-1	68	77
1	3	-6	116	112	5	3	0	102	99	11	3	-3	35	33	3	4	-7	31	37	8	4	3	27	27	4	5	0	38	49
1	3	-5	42	41	5	3	1	86	83	11	3	-2	82	80	3	4	-6	80	79	9	4	-7	26	22	4	5	1	58	51
1	3	-4	47	49	5	3	2	64	74	11	3	-1	34	36	3	4	-5	84	83	9	4	-5	25	32	4	5	2	44	45
1	3	-3	91	93	5	3	3	48	46	11	3	0	37	38	3	4	-4	33	43	9	4	-4	60	69	4	5	3	24	14
1	3	-2	179	185	5	3	4	56	55	11	3	2	23	26	3	4	-3	83	88	9	4	-2	20	39	4	5	4	26	19
1	3	-1	136	156	5	3	5	31	31	12	3	-8	33	24	3	4	-2	71	72	9	4	-1	18	17	5	5	-6	28	25
1	3	0	87	86	6	3	-6	77	70	12	3	-7	21	19	3	4	-1	57	58	9	4	0	27	26	5	5	-5	19	32
1	3	1	101	88	6	3	-5	33	34	12	3	-6	38	37	3	4	0	67	71	9	4	1	25	24	5	5	-3	40	36
1	3	2	37	36	6	3	-3	42	37	12	3	-5	33	28	3	4	2	83	79	9	4	2	33	30	5	5	-2	40	46
1	3	3	46	45	6	3	-1	51	51	12	3	-4	32	32	3	4	3	61	53	10	4	-7	21	16	5	5	2	24	27
1	3	4	42	41	6	3	0	43	42	12	3	-3	35	37	3	4	4	48	48	10	4	-6	19	15	6	5	-6	50	45
1	3	6	42	45	6	3	1	17	13	12	3	-2	41	42	3	4	5	43	40	10	4	-5	22	26	6	5	-3	53	50
1	3	7	21	20	6	3	2	27	28	12	3	-1	98	101	3	4	6	24	21	10	4	-4	38	31	6	5	-1	27	28
2	3	-6	46	44	6	3	3	17	36	12	3	0	62	60	4	4	-8	23	18	10	4	-1	36	53	6	5	1	30	34
2	3	-5	57	56	6	3	4	26	23	12	3	1	23	21	4	4	-7	33	28	11	4	-2	26	36	6	5	2	41	30
2	3	-4	67	70	7	3	-7	16	16	13	3	-8	31	17	4	4	-6	54	52	11	4	-1	35	47	7	5	-6	32	39
2	3	-2	76	75	7	3	-6	31	27	13	3	-6	21	18	4	4	-5	94	96	11	4	0	27	20	7	5	-4	27	29
2	3	-1	57	63	7	3	-5	94	90	13	3	-5	38	38	4	4	-4	104	112	12	4	-1	38	49	7	5	-3	24	18
2	3	0	93	89	7	3	-4	65	58	13	3	-2	42	41	4	4	-3	78	83	13	4	-5	26	24	7	5	-2	24	27
2	3	1	78	74	7	3	-3	52	51	13	3	-1	33	35	4	4	-2	53	65	0	5	-5	25	18	7	5	2	26	20
2	3	2	45	40	7	3	-2	72	70	14	3	-6	24	18	4	4	0	16	12	0	5	-4	61	57	8	5	-5	39	48
2	3	3	59	58	7	3	-1	41	50	14	3	-5	26	9	4	4	1	64	66	0	5	-3	17	16	0	6	-2	38	39
2	3	4	67	61	7	3	0	30	27	14	3	-2	19	24	4	4	2	49	53	0	5	-2	28	33	0	6	-1	44	44
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2	3	7	52	54	7	3	3	34	32	0	4	-6	42	41	4	4	4	39	33	0	5	2	34	33	0	6	1	54	44
3	3	-8	34	39	7	3	4	27	21	0	4	-5	17	10	5	4	-8	25	23	0	5	3	18	16	0	6	2	46	39
3	3	-7	51	56	7	3	5	20	21	0	4	-4	23	23	5	4	-6	44	46	0	5	4	66	57	0	6	3	19	13
3	3	-6	88	88	8	3	-7	51	50	0	4	-3	88	89	5	4	-5	18	22	0	5	5	22	18	1	6	-2	27	26
3	3	-5	94	88	8	3	-6	37	34	0	4	-2	51	51	5	4	-3	68	77	1	5	-5	46	35	1	6	1	22	17
3	3	-4	131	133	8	3	-4	80	72	0	4	0	69	69	5	4	-1	68	71	1	5	-4	23	21	1	6	3	17	6
3	3	-3	98	98	8	3	-3	83	79	0	4	1	16	12	5	4	0	19	26	1	5	-3	47	45	2	6	-3	17	17
3	3	-2	96	97	8	3	-2	80	80	0	4	2	59	51	5	4	1	32	41	1	5	-2	53	56	2	6	1	29	23
3	3	-1	110	111	8	3	-1	144	154	0	4	3	95	89	5	4	2	27	32	1	5	-1	25	26	2	6	2	32	28
3	3	0	72	67	8	3	0	33	33	0	4	4	31	23	5	4	3	53	51	1	5	0	43	47	3	6	1	44	46
3	3	1	13	10	8	3	1	95	97	0	4	6	39	41	6	4	-7	25	20	1	5	1	45	43	4	6	-4	33	31
3	3	2	25	24	8	3	2	28	17	1	4	-5	33	37	6	4	-6	42	49	1	5	2	46	45					
3	3	3	41	38	8	3	3	42	39	1	4	-4	20	27	6	4	-5	55	63	1	5	3	33	28					
3	3	4	34	35	8	3	4	21	28	1	4	-3	63	61	6	4	-4	46	51	1	5	4	21	18					

VI

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
0	0	2	182	-183	6	0	-14	70	-72	13	0	-10	104	-104	3	1	-7	82	74	6	1	2	91	-90	11	1	-4	121	122
0	0	4	315	321	6	0	-12	70	-69	13	0	-8	146	144	3	1	-5	17	-12	6	1	3	42	40	11	1	-3	60	-65
0	0	6	222	-215	6	0	-8	179	179	13	0	-6	114	-113	3	1	-4	51	-54	6	1	6	105	112	11	1	-2	197	196
0	0	8	129	126	6	0	-6	413	-404	13	0	-4	118	-117	3	1	-2	220	206	6	1	7	154	-154	11	1	-1	49	-47
0	0	10	171	170	6	0	-4	254	-251	13	0	-2	167	-158	3	1	-1	93	91	7	1	-14	61	-67	11	1	0	175	177
0	0	12	97	96	6	0	-2	17	-5	14	0	-10	61	61	3	1	0	342	354	7	1	-12	121	-117	11	1	2	87	87
1	0	-10	40	42	6	0	4	189	197	14	0	-8	68	65	3	1	1	31	24	7	1	-11	126	120	12	1	-11	49	-47
1	0	-8	39	-43	6	0	6	219	-229	14	0	-4	125	-121	3	1	2	155	-154	7	1	-10	145	144	12	1	-8	93	-87
1	0	-6	683	-675	7	0	-12	132	131	0	1	1	480	485	3	1	3	25	-29	7	1	-9	49	47	12	1	-6	88	-87
1	0	-4	120	130	7	0	-10	151	153	0	1	2	570	588	3	1	4	231	226	7	1	-7	30	43	12	1	-2	188	187
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1	0	4	81	-78	7	0	-2	513	-524	0	1	6	148	-149	4	1	-10	92	92	7	1	0	24	30	13	1	-7	93	86
1	0	6	384	376	7	0	0	475	468	0	1	8	59	-58	4	1	-8	255	-251	7	1	1	150	157	13	1	-6	87	85
1	0	8	112	109	7	0	2	88	91	0	1	10	117	-118	4	1	-7	52	-55	7	1	3	67	70	13	1	-5	72	-74
1	0	10	259	257	7	0	4	53	46	0	1	11	59	54	4	1	-6	332	-325	7	1	4	287	290	13	1	-4	106	-97
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2	0	-12	155	-155	7	0	8	60	-53	1	1	-10	161	157	4	1	-4	27	-37	8	1	-12	131	-132	14	1	-4	71	-68
2	0	-10	61	-60	8	0	-10	222	216	1	1	-9	41	40	4	1	-3	522	-503	8	1	-11	67	67	14	1	-3	58	-53
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2	0	-4	287	-271	8	0	-4	95	-96	1	1	-7	94	-98	4	1	-1	17	-29	8	1	-8	177	-183	15	1	-4	57	-49
2	0	-2	622	-621	8	0	-2	61	53	1	1	-6	32	37	4	1	0	261	-259	8	1	-6	117	-119	0	2	0	1595	-1532
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2	0	10	179	178	8	0	6	38	33	1	1	-2	304	291	4	1	5	68	-66	8	1	-2	245	-234	0	2	4	249	-247
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5	0	-10	70	-66	11	0	-6	137	-143	2	1	0	307	-303	6	1	-8	88	-85	10	1	-1	78	79	1	2	6	212	-205
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5	0	-6	193	205	11	0	-2	84	-86	2	1	2	87	94	6	1	-6	255	250	10	1	1	79	-75	1	2	8	60	-58
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5	0	-2	44	-50	12	0	-10	122	-115	2	1	4	126	122	6	1	-4	233	-238	10	1	3	50	55	2	2	-13	63	64
5	0	0	17	-32	12	0	-8	127	-128	2	1	6	232	226	6	1	-3	65	-62	11	1	-10	100	94	2	2	-12	89	87
5	0	2	36	-34	12	0	-4	72	66	2	1	8	101	99	6	1	-2	267	258	11	1	-8	157	159	2	2	-10	82	80
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5	0	6	58	57	12	0	0	65	-55	3	1	-9	165	-169	6	1	0	220	223	11	1	-6	56	-61	2	2	-8	93	-100
5	0	8	88	89	13	0	-12	59	-52	3	1	-8	234	-234	6	1	1	85	83	11	1	-5	147	146	2	2	-7	93	-94

Table 4. Continued.

h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc	h	k	l	Fo	Fc
2	2	-6	225	228	9	2	-13	89	92	5	3	-8	135	139	2	4	4	79	79	1	5	-3	49	-58	2	6	7	59	63
2	2	-5	17	-2	9	2	-9	48	51	5	3	-7	76	-70	2	4	5	55	54	1	5	-2	34	37	3	6	-7	123	120
2	2	-4	72	78	9	2	-8	131	-127	5	3	-6	64	65	2	4	7	118	-114	1	5	-1	22	-17	3	6	-6	105	-109
2	2	-3	17	2	9	2	-7	47	-47	5	3	-5	247	256	2	4	8	79	-84	1	5	1	102	107	3	6	-3	80	84
2	2	-2	1323	1347	9	2	-6	116	-118	5	3	-3	91	97	2	4	10	109	-106	1	5	2	49	46	3	6	-2	38	45
2	2	-1	1160	1138	9	2	-5	33	34	5	3	-1	89	91	3	4	-11	52	-59	1	5	4	196	192	3	6	0	52	58
2	2	0	106	-100	9	2	-4	154	-164	5	3	0	146	-141	3	4	-10	62	67	1	5	6	188	-184	3	6	1	43	41
2	2	1	71	76	9	2	-3	195	-191	5	3	1	269	262	3	4	-9	61	-57	2	5	-9	66	71	3	6	2	158	163
2	2	2	215	213	9	2	-2	183	173	5	3	2	82	86	3	4	-8	198	201	2	5	-8	98	-93	3	6	4	96	-96
2	2	3	190	-181	9	2	-1	154	159	5	3	3	38	-23	3	4	-7	60	-60	2	5	-6	77	76	3	6	5	59	59
2	2	4	80	-81	9	2	0	99	-102	5	3	4	53	55	3	4	-6	44	-47	2	5	-4	70	71	4	6	-8	48	-52
2	2	5	93	-91	9	2	1	136	132	5	3	5	115	116	3	4	-5	68	66	2	5	-3	116	-115	4	6	-7	65	69
2	2	6	72	73	9	2	4	136	-134	5	3	6	255	252	3	4	-4	157	-156	2	5	-2	124	-128	4	6	-6	55	-54
2	2	8	98	98	10	2	-12	89	84	6	3	-10	146	-145	3	4	-3	242	-251	2	5	-1	79	87	4	6	-5	54	-59
2	2	9	48	-52	10	2	-10	78	-82	6	3	-7	104	-101	3	4	-2	151	-142	2	5	0	96	-94	4	6	-4	294	-299
2	2	11	76	71	10	2	-9	79	83	6	3	-6	43	-39	3	4	-1	125	-125	2	5	1	102	107	4	6	-1	79	71
3	2	-13	73	68	10	2	-8	96	-91	6	3	-5	125	128	3	4	0	70	-68	2	5	6	53	54	4	6	0	88	-84
3	2	-12	49	51	10	2	-7	76	75	6	3	-3	148	150	3	4	1	101	98	2	5	7	60	58	4	6	1	69	70
3	2	-11	52	51	10	2	-6	92	-90	6	3	-2	187	-188	3	4	2	94	-98	2	5	8	58	55	4	6	3	88	87
3	2	-10	124	-126	10	2	-5	118	-122	6	3	-1	26	10	3	4	3	297	-297	2	5	9	88	-80	4	6	6	80	-76
3	2	-9	85	87	10	2	-3	61	65	6	3	0	209	-199	3	4	4	38	34	3	5	-10	82	-89	5	6	-7	62	-56
3	2	-8	140	-146	10	2	-2	96	88	6	3	1	31	-39	3	4	5	41	-37	3	5	-9	90	92	5	6	-5	61	-65
3	2	-7	226	-226	10	2	0	67	-75	6	3	5	88	92	3	4	6	65	-66	3	5	-6	105	110	5	6	-4	143	-143
3	2	-6	180	176	10	2	1	114	120	6	3	6	107	104	3	4	7	113	-108	3	5	-5	92	-91	5	6	-2	108	-108
3	2	-5	127	-120	10	2	2	153	-150	6	3	7	159	150	3	4	8	111	-111	3	5	-2	53	-57	5	6	-1	75	68
3	2	-4	233	244	11	2	-6	145	147	6	3	8	52	-57	4	4	-10	49	51	3	5	-1	30	-27	5	6	0	43	47
3	2	-3	449	437	11	2	-5	82	-81	7	3	-11	117	-117	4	4	-8	56	56	3	5	0	103	-104	5	6	1	90	-84
3	2	-2	318	325	11	2	-4	98	-102	7	3	-9	89	-95	4	4	-7	30	-22	3	5	1	202	205	5	6	2	76	-88
3	2	-1	241	226	11	2	-3	172	174	7	3	-7	79	-82	4	4	-6	69	-70	3	5	2	74	-72	5	6	4	89	-91
3	2	0	112	112	11	2	-1	70	74	7	3	-5	73	77	4	4	-5	46	-36	3	5	3	91	87	5	6	6	77	-73
3	2	1	17	19	11	2	0	104	-107	7	3	-4	61	-68	4	4	-4	362	374	3	5	5	85	-86	6	6	-7	124	-127
3	2	2	166	-175	12	2	-10	88	94	7	3	0	251	-247	4	4	-3	164	168	3	5	7	49	-51	6	6	-5	83	89
3	2	3	153	156	12	2	-8	75	80	7	3	1	120	-126	4	4	-2	248	251	3	5	8	77	71	6	6	-2	86	88
3	2	4	295	285	12	2	-3	62	63	7	3	3	77	-71	4	4	-1	165	-165	4	5	-8	100	-94	6	6	1	65	-58
3	2	6	76	76	13	2	-6	96	90	7	3	4	144	-149	4	4	0	173	169	4	5	-5	355	-367	6	6	4	81	-81
3	2	7	127	123	13	2	-2	99	95	7	3	5	52	64	4	4	1	80	-82	4	5	-4	233	-242	6	6	5	59	-56
3	2	8	163	159	15	2	-5	67	-54	8	3	-12	83	83	4	4	2	31	-36	4	5	-3	108	118	7	6	-7	53	-49
3	2	10	59	54	0	3	1	303	-288	8	3	-11	87	-91	4	4	3	79	-75	4	5	-2	64	56	7	6	-6	139	137
4	2	-12	81	-79	0	3	3	75	-77	8	3	-8	179	176	4	4	5	52	-46	4	5	1	152	152	7	6	-3	62	-69
4	2	-11	83	88	0	3	4	35	32	8	3	-7	128	-127	4	4	6	68	-65	4	5	2	45	-40	7	6	-2	57	59
4	2	-9	85	-81	0	3	5	41	33	8	3	-5	147	-141	4	4	9	83	-75	4	5	3	52	-54	7	6	-1	64	60
4	2	-8	82	-90	0	3	6	44	39	8	3	-4	176	175	5	4	-8	108	-116	4	5	5	89	-90	7	6	0	104	-102
4	2	-7	69	-65	0	3	8	111	113	8	3	-2	60	66	5	4	-7	100	108	4	5	6	65	-70	7	6	3	78	-78
4	2	-6	74	70	1	3	-9	43	-46	8	3	-1	87	-93	5	4	-5	140	145	4	5	8	87	-83	8	6	-8	74	78
4	2	-5	116	114	1	3	-7	41	-44	8	3	0	39	-32	5	4	-4	159	165	5	5	-11	71	62	8	6	-6	83	78
4	2	-4	247	-229	1	3	-6	94	-92	8	3	1	82	-84	5	4	-2	218	218	5	5	-10	85	87	8	6	-3	43	38
4	2	-3	172	163	1	3	-5	153	149	8	3	2	87	84	5	4	-1	74	-70	5	5	-9	125	-128	8	6	-2	43	-43
4	2	-2	194	-186	1	3	-4	78	-78	9	3	-12	58	52	5	4	0	97	93	5	5	-6	35	-38	8	6	3	112	-110
4	2	-1	26	21	1	3	-3	145	148	9	3	-8	82	79	5	4	1	88	-87	5	5	-5	185	-190	9	6	-4	59	-63
4	2	0	151	-156	1	3	-2	229	-226	9	3	-7	42	-33	5	4	2	44	39	5	5	-1	44	-39	9	6	-3	124	118
4	2	1	43	-41	1	3	-1	215	-190	9	3	-6	95	94	5	4	3	141	143	5	5	0	38	-35	9	6	-1	51	-57
4	2	3	35	27	1	3	0	58	-61	9	3	-4	142	-147	5	4	5	40	37	5	5	1	54	-61	11	6	-4	76	-71
4	2	5	104	-104	1	3	1	252	-261	9	3	-2	73	84	5	4	6	46	46	5	5	2	39	-31	0	7	2	106	-115
4	2	6	89	88	1	3	2	82	83	9	3	-1	130	-138	5	4	8	108	104	5	5	5	108	-104	0	7	4	70	-74
4	2	7	142	143	1	3	3	173	162	9	3	0	110	117	6	4	-9	73	79	5	5	6	100	-102	0	7	6	55	56
4	2	9	123	122	1	3	4	43	-43	9	3	1	111	-117	6	4	-8	132	-138	6	5	-10	82	84	1	7	-7	78	74
5	2	-11	60	-68	1	3	5	126	-129	9	3	2	228	233	6	4	-7	154	156	6	5	-6	229	234	1	7	-5	86	-88
5	2	-10	83	82	1	3	6	29	-28	9	3	4	46	41	6	4	-5	110	106	6	5	-5	49	57	1	7	-4	86	89
5	2	-9	117	-121	1	3	8	95	-97	10	3	-6	101	-107	6	4	-4	55	-48	6	5	-4	63	55	1	7	-2	43	48
5	2	-7	73	-67	1	3	9	129	-127	10	3	-5	75	75	6	4	-3	54	43	6	5	-3	143	-137	1	7	2	51	-54
5	2	-6	72	-65	1	3	10	86	86	10	3	-4	121	-127	6	4	-2	63	-60	6	5	-2	120	110	1	7	4	54	-55
5	2	-3	182	178	1	3	11	57	-53	10	3	-1	42	-54	6	4	-1	43	-35	6	5	1	43	-48	1	7	5	118	116
5	2	-2	106	-101	2	3	-9	112	-121	10	3	0	126	130	6	4	1	132	139	6	5	4	71	70	1	7	6	88	91
5	2	-1	164	164	2	3	-8	98	95	10	3	3	77	-71	6	4	4	62	-56	6	5	5	130	-125	2	7	-4	86	92
5	2	0	249	-256	2	3	-7	22	25	11	3	-10	80	-71	6	4	5	50	43	7	5	-9	61	64	2	7	-1	45	-42
5	2	1	153	-147	2	3	-6	175	-170	11	3	-8	53	-63	6	4	6	124	124	7	5	-7	78	77	3	7	-8	56	60
5	2	2	133	129	2	3	-5	142	137	11	3	-6	117	-124	7	4	-7	120	127	7	5	-6	84	83	3	7	-7	57	-56
5	2	3	196	-191	2	3	-4	439	-436	11	3	-5	83	-85	7	4	-6	96	-92	7	5	-4	84	81	3	7	-5	45	38
5	2	6	36	-32	2	3	-3	431	-427	11	3	-4	81	84	7	4	-5	61	62	7	5	-2	143	-141	3	7	-3	67	-66
5	2	7	133	105	2	3	-2	55	53	11	3	-3	54	49	7	4	-4	70	-63	7	5	-1	91	88	3	7	1	56	-52
5	2	8	100	-101	2	3	-1	157	169	11	3	-2	73	-72	7	4	-3	96	94	7	5	0	214	209	3	7	2	62	66
6	2	-9	135	-135	2	3	0	260	254	11	3	-1	83	80	7	4	-1	66	-62	7	5	1	64	-76	4	7	-5	79	77
6	2	-8	22	27	2	3	1	74	-74	11	3	0	81	-87	7	4	1	53	62	7	5	2	79	82	4	7	-3	77	-76
6	2	-7	47	42	2	3	2	20	21	11	3	2	80	-84	7	4	2	90	-92	7	5	4	137	134	4	7	-2	68	59
6	2	-6	194	204	2	3	3	164	157	12	3	-6	68	61	7	4	3	149	148	8	5	-7	104	101	4	7	6	75	71
6	2	-5	181	-178	2	3	4	182	-183	12	3	0	122	-120	7	4	5	58	47	8	5	-5	80	87	5	7	-4	56	-51
6	2	-4	100	96	2	3	5	54	52	13	3	-6	85	73	7	4	6	64	-69	8	5	-4	124	-127	5	7	-1	100	98
6	2	-3	142	-148	2	3	6	125	-125	13	3	-4	52	45	8	4	-7	94	99	8	5	-1	57	49	5	7	2	61	63
6	2	-1	53	-51	2	3	8	207	-205	14	3	-4	66	61	8	4	-6	67	-62	8	5	3	82	80	6	7	-7	89	-94
6	2	0	38	34	2	3	9	68	-70	0	4	0	20	31	8	4	-5	46	38	8	5	4	68	64	6	7	-6	169	-174
6	2	1	133	-125	2	3	10	82	77	0	4	1	147	148	8	4	-3	107	-113	9	5	-5	60	62	6	7	-5	67	67
6	2	3	141	-142	3	3	-10	156	156	0	4	2	182	184	8	4	2	124	-130	9	5	-3	114	-114	6	7	-3	65	62
6	2	4	32	32	3	3	-9	89	87	0	4	3	149	144	8	4	3	149	148	9	5	0	91	-91	6	7	-2	56	-56
6	2	5	195	196	3	3	-8	85	-84	0	4	4	153	143	8	4	4	85	90	9	5	2	136	-129	6	7	4	55	-57
6	2	7	73	-65	3	3	-6	103	-97	0	4	7	156	-157	9	4	-8	80	77	10	5	-8	57	-59	7	7	-6	89	-92
7	2	-13	95	-91	3	3	-5	96	94	0	4	8	56	57	9	4	-4	184	193	10	5	-6	49	52	7	7	-2	61	60
7	2	-10	76	-86	3	3	-3	25	-19	0	4	10	97	96	9	4	-3	59	-58	10	5	-4	73	74	7	7	-1	142	-142
7	2	-9	89	86	3	3	-1	63	-55	1	4	-12	79	-78	9	4	-2	281	-278	10	5	0	61	-61	7	7	2	87	-91
7	2	-8	55	60	3	3	0	124	119	1	4	-8	184	-188	9	4	1	86	-81	10	5	1	78	77	8	7	-4	51	54
7	2	-6	83	88	3	3	1	189	-197	1	4	-7	32	36	9	4	3	45	41	11	5	-5	86	-82	0	8	0	87	95
7	2	-5	57	-66	3	3	2	86	92	1	4	-6	85	79	9	4	4	72	78	11	5	1	74	65	0	8	1	63	-63
7	2	-4	138	200	3	3	3	128	-133	1	4	-5	44	-41	10	4	-9	119	-121	0	6	0	192	-189	1	8	-5	94	94
7	2	-3	51	-48	3	3	4	213	-210	1	4	-3	144	-145	10	4	-8	52	54	0	6	1	130	-133	1	8	-1	70	70
7	2	-2	164	157	3	3	5	170	163	1	4	-1	52	56	10	4	-7	58	-65	0	6	2	53	53	1	8	5	78	78
7	2	-1	281	-275	3	3	7	52	47	1	4	0	75	81	10	4	-6	86	88	0	6	3	75	-75	2	8	-5	55	55
7	2	0	115	-116	3	3	8	154	-150	1	4	1	43	46	10	4	-3	49	-43	0	6	4	71	-70	2	8	0	80	-76
7	2	3	99	-103	4	3	-10	89	-89	1	4	2	30	28	10	4	-2	44	-49	0	6	6	102	101	2	8	2	72	-71
7	2	6	169	178	4	3	-8	164	171	1	4	3	230	231	10	4	2	79	85	0	6	7	68	66	2	8	5	77	84
8	2	-10	90	-94	4	3	-7	50	55	1	4	4	45	80	11	4	-6	75	-76	1	6	-8	114	118	3	8	-6	62	61
8	2	-9	140	136	4	3	-6	50	-55	1	4	6	63	61	11	4	0	129	127	1	6	-7	122	-123	4	8	-6	54	57
8	2	-8	89	-85	4	3	-5	162	171	1	4	10	76	72	12	4	-6	69	-68	1	6	-4	58	-54	4	8	-4	72	69
8	2	-7	117	-124	4	3	-4	688	681	2	4	-10	90	-91	12	4	-5	51	45	1	6	-3	87	94	4	8	-3	53	-55
8	2	-6	40	-32	4	3	-3	374	384	2	4	-8	80	82	12	4	1	73	-66	1	6	-1	85	-86	4	8	8	69	59
8	2	-5	51	-59	4	3	-2	274	-277	2	4	-7	68	-62	0	5	1	59	-59	1	6	4	95	91	5	8	-4	108	103
8	2	-4	56	47	4	3	0	131	125	2	4	-6	144	-151	0	5	2	83	77	1	6	5	68	-67	5	8	1	101	102
8	2	-2	29	13	4	3	1	183	-188	2	4	-5	22	22	0	5	3	64	59	2	6	-7	53	59	5	8	2	70	-70
8	2	-1	48	53	4	3	3	74	71	2	4	-3	297	-300	0	5	5	92	87	2	6	-5	36	-32	6	8	-5	91	-96
8	2	0	111	-111	4	3	4	81	80	2	4	-2	796	-775	0	5	6	51	-50	2	6	-3	105	107	6	8	-4	58	51
8	2	1	83	-78	4	3	5	114	114	2	4	-1	53	-48	0	5	7	35	-38	2	6	-2	103	104	6	8	-1	64	59
8	2	2	58	62	4	3	7	111	-108	2	4	0	86	89	0	5	8	87	-84	2	6	-1	110	-111					
8	2	3	90	87	4	3	8	111	108	2	4	1	122	-125	0	5	9	66	72	2	6	0	147	148					
8	2	5	163	-167	5	3	-11	66	68	2	4	2	76	-80	1	5	-7	64	65	2	6	2	83	84					
					5	3	-10	196	-196	2	4	3	136	139	1	5	-6	69	-64	2	6	5	70	-68					

Table 5. The principal axes of the thermal vibration ellipsoids given by the components of a unit vector in fractional coordinates e_x, e_y, e_z; the corresponding r.m.s. amplitudes, and the B-values.

Atom	e_x	e_y	e_z	$(\overline{u^2})^{\frac{1}{2}}$ Å	B(Å^2)
		(II)			
S	.069	.028	−.176	.249	4.88
	.093	−.038	.116	.241	4.57
	.016	.100	.092	.200	3.15
O	.084	−.002	.159	.251	4.99
	.081	.001	−.166	.228	4.11
	.001	.111	.004	.166	2.16
N	.102	.005	.112	.249	4.90
	−.057	.017	.198	.222	3.88
	.004	.109	−.036	.167	2.21
C1	.085	.006	.157	.236	4.42
	.010	.109	−.038	.191	2.88
	−.079	.020	.163	.181	2.59
C2	.068	.035	.173	.277	6.07
	−.094	.012	.133	.231	4.21
	.012	−.104	.073	.201	3.20
C3	.075	.068	.105	.298	7.03
	−.089	.057	.090	.237	4.43
	.001	−.067	.184	.214	3.61
C4	−.006	.109	.035	.253	5.04
	.016	.017	−.225	.237	4.44
	.115	.003	.033	.220	3.83
C5	.080	−.022	.161	.268	5.68
	−.081	.013	.164	.222	3.90
	.026	.108	.013	.198	3.11
C6	.098	.001	.126	.245	4.74
	.063	.013	−.191	.188	2.78
	−.009	.110	.022	.183	2.65
C7	.097	−.006	.127	.255	5.13
	.050	.077	−.132	.191	2.87
	−.041	.079	.139	.180	2.56
		(III)			
O1	.076	.110	.030	.308	7.49
	.110	−.180	.011	.300	7.12
	.122	.093	−.015	.253	5.04
O2	.007	−.064	.003	.291	6.70
	−.070	.203	.006	.263	5.46
	.167	.088	.011	.221	3.87

Table 5. Continued.

N	.002	.153	−.025	.272	5.86
	.012	.172	.023	.232	4.24
	.181	−.014	.008	.224	3.96
C1	.002	−.096	.031	.276	6.02
	.174	.060	.012	.225	3.98
	−.051	.201	.011	.211	3.52
C2	.058	.097	−.026	.303	7.24
	−.072	.201	.006	.246	4.76
	.156	.057	.023	.235	4.37
C3	.163	.091	.002	.286	7.45
	.053	−.049	.034	.275	5.99
	−.059	.206	.007	.240	4.53
C4	.104	−.037	.033	.303	7.27
	.139	.106	−.008	.248	4.86
	−.054	.201	.010	.240	4.56
C5	.025	−.119	.030	.297	6.97
	−.084	.166	.013	.232	4.25
	.158	.107	.013	.226	4.02
C6	.001	−.119	.029	.272	5.83
	.162	.089	.016	.224	3.98
	−.081	.176	.012	.195	3.01
C7	.031	−.120	.030	.281	6.24
	.136	.143	.015	.250	4.92
	−.116	.135	.011	.226	4.03
CM	.028	.209	−.012	.316	7.90
	−.105	.093	.019	.267	5.62
	.145	.027	.027	.249	4.89
			(IV)		
O1	.159	−.106	.003	.336	8.93
	.106	.061	−.037	.293	6.78
	.118	.087	.030	.208	3.42
O2	−.162	.051	.029	.258	5.26
	.137	−.016	.037	.226	4.05
	.074	.140	−.006	.214	3.63
N	.169	.098	−.004	.255	5.14
	−.110	.096	.028	.238	4.47
	.099	−.060	.038	.198	3.11
C1	.073	.019	.045	.221	3.87
	.043	.145	−.009	.216	3.67
	−.208	.037	.014	.197	3.06
C2	.001	.144	.014	.271	5.80
	.140	.034	−.036	.238	4.46
	.175	−.027	.029	.209	3.46

Table 5. Continued.

C3	.027	−.131	.023	.315	7.82
	−.128	.050	.036	.238	4.46
	.182	.055	.022	.206	3.36
C4	.078	−.074	.038	.323	8.22
	−.151	.069	.028	.226	4.03
	.147	.111	.008	.209	3.43
C5	.129	.022	.038	.285	6.41
	.091	.121	−.021	.224	3.95
	−.160	.086	.019	.209	3.46
C6	.121	.062	.035	.227	4.08
	.034	.122	−.027	.219	3.77
	−.186	.063	.018	.181	2.59
C7	.102	−.129	.012	.249	4.90
	.186	.046	−.022	.236	4.41
	.072	.062	.041	.211	3.51
			(V)		
O	.046	.145	.055	.263	5.46
	−.037	.027	.069	.220	3.82
	.055	−.105	.094	.189	2.81
N1	.003	.177	−.021	.274	5.94
	.068	.014	.112	.222	3.89
	−.043	.035	.059	.196	3.03
N2	.028	.168	.033	.261	5.40
	.006	−.024	.116	.203	3.25
	.075	−.061	.045	.192	2.91
C1	.016	−.176	.019	.233	4.27
	.067	.037	.110	.204	3.29
	.041	.010	−.063	.187	2.76
C2	−.011	.177	.008	.256	5.19
	.050	.035	−.045	.223	3.92
	.062	.002	.120	.205	3.33
C3	.018	−.175	.029	.288	6.55
	.077	.033	.033	.244	4.70
	.017	.033	.121	.198	3.10
C4	.016	−.154	.067	.271	5.78
	.076	.053	.074	.246	4.79
	−.020	.078	.081	.197	3.05
C5	.013	.173	.036	.265	5.54
	.036	−.051	.123	.242	4.64
	.071	−.007	.002	.210	3.47
C6	−.004	.157	.052	.225	4.00
	.003	−.089	.099	.204	3.28
	.080	.011	.063	.185	2.70

Table 5. Continued.

C7	.005	.178	.021	.224	3.98
	.003	.026	−.108	.216	3.67
	.080	−.012	.066	.188	2.79
C8	.037	−.144	.073	.287	6.50
	.028	.103	.105	.224	3.96
	.066	.035	−.009	.218	3.77
C9	.025	.172	.016	.241	4.60
	.073	−.055	.027	.207	3.40
	.022	−.010	.125	.190	2.84
C10	.015	.119	−.057	.250	4.93
	.008	.125	.086	.224	3.96
	.076	−.053	.077	.217	3.71
C11	.044	.150	.047	.298	7.01
	.022	−.055	.119	.262	5.42
	.063	−.085	.005	.204	3.30
C12	.013	.168	.037	.306	7.39
	.022	−.065	.117	.252	5.02
	.076	−.011	.025	.215	3.65
C13	−.029	.003	.082	.276	6.01
	.035	−.160	.048	.248	4.87
	.067	.084	.087	.220	3.82
C14	.006	.152	−.055	.269	5.71
	.077	−.038	.039	.236	4.41
	.022	.090	.109	.209	3.46
CM	.010	.142	.076	.287	6.49
	.058	.063	−.022	.234	4.31
	.055	−.092	.101	.188	2.80
		(VI)			
O	−.039	.104	.017	.259	5.30
	.059	.013	.079	.220	3.81
	.040	.081	−.034	.185	2.71
N1	−.033	.097	.032	.264	5.50
	.065	.076	.012	.220	3.83
	.036	−.049	.081	.174	2.39
N2	.072	−.061	.018	.231	4.20
	.025	.044	.083	.223	3.93
	.030	.109	−.023	.182	2.61
C1	−.043	.102	.011	.227	4.06
	.040	−.007	.087	.208	3.43
	.056	.084	−.006	.193	2.95
C2	.038	−.116	.007	.279	6.15
	.035	.017	.087	.253	5.07
	.063	.061	−.010	.194	2.99

Table 5. Continued.

C3	.003	−.124	.030	.274	5.94
	−.012	.046	.061	.251	4.99
	.080	.011	.042	.205	3.30
C4	.051	.073	−.025	.267	5.63
	.004	.090	.062	.234	4.32
	.063	−.064	.058	.204	3.29
C5	.067	.025	−.017	.232	4.25
	.022	.094	.062	.225	4.01
	.041	−.090	.060	.207	3.40
C6	.026	−.071	.074	.218	3.75
	−.063	.043	.018	.198	3.10
	.044	.103	.043	.186	2.74
C7	.074	−.016	.063	.232	4.26
	−.019	.088	.050	.208	3.40
	.029	.098	−.036	.171	2.31
C8	−.047	.084	.023	.243	4.64
	.066	.052	.063	.227	4.08
	.007	.089	−.058	.192	2.92
C9	.075	−.039	.010	.226	4.05
	.030	.057	.079	.216	3.68
	.011	.113	−.036	.176	2.43
C10	.077	−.031	.011	.252	5.02
	.024	.123	.028	.236	4.38
	.014	−.038	.083	.204	3.27
C11	−.059	.071	.012	.296	6.93
	.044	.110	.008	.255	5.13
	.035	−.019	.087	.210	3.47
C12	−.026	.053	.059	.299	7.08
	.050	−.103	.009	.252	4.99
	.059	−.063	.064	.213	3.59
C13	.026	.020	.087	.277	6.07
	.055	.087	−.005	.258	5.27
	.054	−.098	.013	.217	3.72
C14	.080	−.012	.020	.259	5.30
	.001	−.019	.047	.223	3.92
	.014	.075	.072	.219	3.79

linked by bonds (of length 2.980 Å) between heterocyclic and amino nitrogens. This type of hydrogen bond occurs also in adenosine,[19] but is there much longer (3.133 Å). Other bond lengths reported [25] show that the value 2.933 Å corresponds to a strong hydrogen bond of this type.

The considerable change in geometry of the heterocyclic part of (VI) with respect to (V) (and the others) are probably related to the hydrogen bonds.

Table 6. Bond distances and angles with estimated standard deviations.

Distance	(Å)		Distance	(Å)	
	(I)	(II)		(I)	(II)
S–C7	1.629(7)	1.643(3)	C2–C3	1.370(12)	1.396(11)
O–C7	1.393(9)	1.369(8)	C3–C4	1.368(13)	1.387(6)
N–C7	1.354(8)	1.347(8)	C4–C5	1.397(13)	1.381(10)
O–C1	1.414(8)	1.383(7)	C5–C6	1.374(10)	1.385(10)
N–C6	1.404(9)	1.398(8)	C6–C1	1.375(10)	1.390(5)
C1–C2	1.390(12)	1.352(9)	N–CM	1.470(9)	–

Angle	(°)		Angle	(°)	
	(I)	(II)		(I)	(II)
S–C7–O	123.1(5)	122.8(4)	N–C6–C5	133.2(7)	134.1(6)
S–C7–N	129.5(6)	129.7(5)	C1–C2–C3	114.1(8)	115.6(6)
O–C7–N	107.3(6)	107.5(3)	C2–C3–C4	121.7(8)	121.8(9)
C7–O–C1	108.5(5)	108.6(3)	C3–C4–C5	123.3(8)	121.7(9)
C7–N–C6	109.6(6)	110.5(4)	C4–C5–C6	116.2(8)	116.5(7)
O–C1–C6	106.9(6)	108.3(6)	C5–C6–C1	119.0(7)	120.7(7)
N–C6–C1	107.8(6)	105.2(6)	C6–C1–C2	125.7(7)	123.7(7)
O–C1–C2	127.4(7)	128.1(5)	C6–N–CM	125.5(6)	–
			C7–N–CM	124.9(6)	

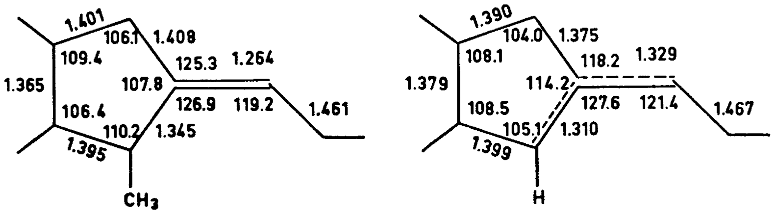
Distance	(Å)		Distance	(Å)	
	(III)	(IV)		(III)	(IV)
O1–C7	1.210(2)	1.211(3)	C2–C3	1.397(3)	1.380(4)
O2–C7	1.379(2)	1.368(3)	C3–C4	1.380(3)	1.375(4)
N–C7	1.355(2)	1.346(3)	C4–C5	1.384(3)	1.383(4)
O2–C1	1.390(2)	1.386(2)	C5–C6	1.382(3)	1.385(3)
N–C6	1.388(2)	1.390(3)	C6–C1	1.373(2)	1.366(3)
C1–C2	1.360(3)	1.374(3)	N–CM	1.441(2)	–

Angle	(°)		Angle	(°)	
	(III)	(IV)		(III)	(IV)
O1–C7–O2	122.2(2)	121.7(2)	N–C6–C5	132.9(2)	133.7(2)
O1–C7–N	129.7(2)	129.9(2)	C1–C2–C3	116.5(2)	116.0(3)
O2–C7–N	108.1(2)	108.4(2)	C2–C3–C4	120.7(2)	121.5(2)
C7–O2–C1	107.2(1)	106.8(2)	C3–C4–C5	122.0(2)	121.9(2)
C7–N–C6	109.5(1)	109.8(2)	C4–C5–C6	116.8(2)	116.6(3)
O2–C1–C6	108.8(2)	109.5(2)	C5–C6–C1	120.7(2)	120.8(2)
N–C6–C1	106.4(1)	105.5(2)	C6–C1–C2	123.3(2)	123.2(2)
O2–C1–C2	127.9(2)	127.3(2)	C6–N–CM	126.4(2)	–
			C7–N–CM	124.1(2)	–

Table 6. Continued.

Distance	(Å)		Distance	(Å)	
	(V)	(VI)		(V)	(VI)
N1 – C7	1.264(5)	1.329(3)	C6 – C1	1.365(6)	1.379(3)
O – C7	1.408(4)	1.375(3)	N2 – CM	1.453(6)	–
N2 – C7	1.345(5)	1.310(3)	N1 – C8	1.461(6)	1.467(3)
O – C1	1.401(5)	1.390(3)	C8 – C9	1.524(6)	1.502(4)
N2 – C6	1.395(5)	1.399(3)	C9 – C10	1.371(6)	1.382(4)
C1 – C2	1.369(5)	1.366(4)	C10 – C11	1.396(6)	1.376(4)
C2 – C3	1.395(7)	1.379(4)	C11 – C12	1.365(8)	1.381(4)
C3 – C4	1.366(7)	1.395(4)	C12 – C13	1.357(7)	1.373(4)
C4 – C5	1.399(6)	1.387(4)	C13 – C14	1.392(6)	1.375(4)
C5 – C6	1.377(6)	1.381(3)	C14 – C9	1.381(6)	1.394(4)

Angle	(°)		Angle	(°)	
	(V)	(VI)		(V)	(VI)
N1 – C7 – O	125.3(4)	118.2(2)	C6 – C1 – C2	124.0(4)	123.9(2)
N1 – C7 – N2	126.9(4)	127.6(2)	C6 – N2 – CM	126.4(4)	–
O – C7 – N2	107.8(3)	114.2(2)	C7 – N2 – CM	123.3(4)	–
C7 – O – C1	106.1(3)	104.0(2)	C7 – N1 – C8	119.2(4)	121.4(2)
C7 – N2 – C6	110.2(3)	105.1(2)	N1 – C8 – C9	113.0(4)	110.3(2)
O – C1 – C6	109.4(3)	108.1(2)	C8 – C9 – C10	119.3(4)	121.2(2)
N2 – C6 – C1	106.4(4)	108.5(2)	C8 – C9 – C14	121.5(4)	121.3(2)
O – C1 – C2	126.6(4)	128.0(2)	C9 – C10 – C11	120.1(5)	121.5(3)
N2 – C6 – C5	132.5(4)	131.7(2)	C10 – C11 – C12	120.2(5)	120.3(3)
C1 – C2 – C3	115.5(5)	116.7(3)	C11 – C12 – C13	120.1(5)	119.0(3)
C2 – C3 – C4	121.0(4)	120.2(3)	C12 – C13 – C14	120.3(5)	120.6(3)
C3 – C4 – C5	122.8(5)	122.2(3)	C13 – C14 – C9	120.1(5)	121.1(3)
C4 – C5 – C6	115.6(5)	117.0(3)	C14 – C9 – C10	119.2(4)	117.4(3)
C5 – C6 – C1	121.1(4)	119.8(2)			


1.401
106.1
1.408
109.4
125.3
1.264
1.365
107.8
106.4
126.9
119.2
1.461
110.2
1.345
1.395
CH3
1.390
104.0
1.375
108.1
118.2
1.329
1.379
114.2
108.5
127.6
121.4
1.467
105.1
1.310
1.399
H

(V) (VI)

Fig. 2.

C7 – N1 is longer, in fact even longer than C7 – N2, which, on the other hand, is significantly shorter than in (V). The effect on the O – C7 bond is the same (see Fig. 2). Together with these changes in bond lengths, there are corresponding differences in angles. The angle O – C7 – N2 is opened by 6.4°, while C1 – O – C7 and C7 – N2 – C6 are 2.1° and 5.1° smaller, respectively. In agreement with the longer bond, the C7 – N1 stretching frequency of (VI) has recently been determined [26,27] to bee about 1650 cm^{-1}.

The C = S distances (1.629 Å) and (1.643 Å) agree within error limits with the value obtained for 1,3-dithiolane-2-thione (1.652 Å),[20] but is significantly shorter than that of ethylenethiourea (1.708 Å).[21] 1.210 Å and 1.211 Å for C = O bonds correspond to the value of 1.211 Å in 2-oxazolidinone,[22] which, however, has a considerably shorter N – C7 bond (1.304 Å). The O – C7 bond of 2-oxazolidinone is also shorter (1.354 Å) than in the benzoxazoline derivatives. The angles C – O – C, C – N – C and O – C – N of the heterocyclic ring resemble those of *N*-methyl-5,5-dimethyl-oxazolidine-2,5-dione,[23] and also the N – C(methyl) single bond distance of this compound (1.461 Å) agrees with the values of (I), (III), and (V). The geometry around the central bond, C1 – C6, corresponds to that of 2-acetyl-3-indazolinone.[24]

Bond distances and angles in the benzylidene parts of (V) and (VI) have normal values.

Except for the hydrogen bond in (VI), no short intermolecular contacts have been observed.

Acknowledgement. The author would like to thank Dr. K. Davidkov* for supplying the compounds and preparing the crystals.

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Received October 12, 1972.