

The Crystal Structure of *anti-p*-Chlorobenzaldoxime

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The crystal structure of *anti-p*-chlorobenzaldoxime, $\text{Cl}-\text{C}_6\text{H}_4-\text{CH}=\text{NOH}$, has been determined from three-dimensional X-ray intensity data collected on a Stoe-Güttinger Weissenberg diffractometer. The structure has been refined by full-matrix least-squares methods to give a final *R*-value of 0.06. The positions of all hydrogen atoms were revealed by a difference-Fourier synthesis calculated from structure factors with $\sin\theta/\lambda < 0.35$.

A comparison of the intramolecular geometry with those found for other benzenoid aldoximes, especially that of *syn-p*-chlorobenzaldoxime, indicates that the difference in steric strain between the two isomers is not reflected in the bonding system or by the majority of the angles. However, the angle $\angle\text{C}-\text{C}=\text{N}$ is increased, from the 121° found in *syn-p*-chlorobenzaldoxime, to 132° in the present compound.

A rather short intramolecular contact of 2.82 Å is found between the oxime oxygen atom and a ring carbon atom.

This paper reports a three-dimensional crystal structure analysis of *anti-p*-chlorobenzaldoxime. The structure has been solved in two projections by Jerslev.¹ The primary aim of the reinvestigations was to obtain intramolecular dimensions for this compound to the same degree of accuracy as those obtained for *syn-p*-chlorobenzaldoxime, *anti-p*-chloro-*N*-methylbenzaldoxime, and *anti*-2,6-dimethyl-4-chloro-*N*-methylbenzaldoxime (Folting *et al.*,² Gram Jensen and Jerslev³) in order to examine how the intramolecular dimensions of the *p*-chlorobenzaldoximes are affected by small changes in the molecular skeleton. A short account of the results was presented at the IUC Congress in USA (Gram Jensen⁴).

EXPERIMENTAL

anti-p-Chlorobenzaldoxime crystallizes from an alcohol-water solutions as long, usually flat, needles, elongated in the *b* direction. The faces [001] and [101] are well developed, while the faces [102] show up in a few cases only. The space group is $P2_12_12_1$, the number of molecules in the unit cell is 4, and the density measured by flotation is $1.43 \text{ g}\cdot\text{cm}^{-3}$ (Jerslev¹). The unit cell constants derived from precession photographs (MoK α , $\lambda=0.71069 \text{ \AA}$) are: $a=6.547$, $b=4.641$, $c=23.37 \text{ \AA}$, with a relative standard

deviation of 0.2 %, estimated from repeated measurements, The calculated density is $1.45 \text{ g} \cdot \text{cm}^{-3}$.

Intensity data were collected by means of an automatic Weissenberg diffractometer (delivered by Stoe & Cie. GmbH, Darmstadt, West Germany) using $\text{MoK}\alpha$ radiation with a LiF monochromator. Harmonics were excluded by using a scintillation detector with proper settings of a pulse height discriminator. A needle-shaped crystal of dimensions $0.5 \times 1.25 \times 0.5 \text{ mm}^3$ was used with the needle axis (b -axis) as rotation axis. All the symmetry allowed reflexions $h0l$ through $h4l$ were measured using the ω -scan method. The constancy of the primary beam and the counting system was checked by frequent re-measurement of a standard reflexion.

The internal consistency of the diffractometer output was checked, and the net reflected intensities and their standard deviations (based on counting statistics) were calculated by means of the ALGOL program PDR. Using the FORTRAN program LP, the reflexions with net intensities less than twice their standard deviation were rejected, and the remaining 722 were converted to structure factors using the conventional L_p correction formulas. No corrections for absorption were applied ($\mu_{\text{Mo}} = 4.5 \text{ cm}^{-1}$).

The calculations were carried out on the IBM 7090/94 computer at NEUCC and on the GIER computer, both situated at the Technical University of Denmark.

STRUCTURE ANALYSIS

The several calculations needed for the regular structure analysis were performed by means of the system of X-RAY 63 crystallographic programs edited by J. Stewart, the University of Maryland. The atomic scattering factors used were those given in Volume III of *International Tables of Crystallography*, 1962. For the non-hydrogen atoms an isotropic temperature factor $B = 4.0 \text{ \AA}^2$, and the coordinates obtained by Jerslev,¹ were used as starting parameters. A series of full-matrix least-squares refinements was carried out, applying the weights $w = 1/\sigma(F_o^2)$. All observed structure factors were included in the initial series of isotropic refinement. After refinement of the scale factor only, the R value was 0.18 (weighted $R = 0.23$). Several further cycles, in which all positional and isotropic thermal parameters were refined, reduced R to 0.15 (weighted $R = 0.17$). In order to eliminate the influence from the hydrogen atoms, 161 reflexions with $\sin\theta/\lambda < 0.35$ were omitted from the next step of refinement, in which anisotropic thermal parameters were introduced. This lowered the R value to 0.08 (weighted $R = 0.10$).

The positions of the hydrogen atoms were revealed from a three-dimensional difference-Fourier synthesis calculated from structure factors with $\sin\theta/\lambda < 0.35$. All the hydrogen atoms appeared clearly, and no spurious peaks were seen.

Next, the least squares refinement was recontinued. The thermal movements of the hydrogen atoms were approximately accounted for by a fixed isotropic B parameter equal to 3.0 \AA^2 . All the observed structure factors were included in this final refinement, which proceeded in three stages, each consisting of two cycles: the anisotropic thermal parameters and the positional parameters of all non-hydrogen atoms were refined in the first and second stage, respectively. The positional parameters of the hydrogen atoms were refined in the third stage. The final R value was 0.06 (weighted $R = 0.07$).

A list of observed and calculated structure factors are given in Table 7. Final fractional atomic coordinates, and the final thermal parameters, are listed in Tables 1 and 2.

Table 1. Fractional atomic coordinates and standard deviations.

Atom	<i>x</i>	$\sigma(x)$	<i>y</i>	$\sigma(y)$	<i>z</i>	$\sigma(z)$
Cl	1.0004	(3)	0.3201	(4)	0.0530	(1)
C1	0.7845	(8)	0.4437	(11)	0.0886	(2)
C2	0.6665	(9)	0.6535	(13)	0.0633	(2)
C3	0.4916	(10)	0.7461	(11)	0.0912	(2)
C4	0.4382	(8)	0.6355	(10)	0.1448	(2)
C5	0.5644	(9)	0.4270	(13)	0.1693	(2)
C6	0.7369	(8)	0.3341	(13)	0.1417	(2)
C7	0.2523	(9)	0.7532	(11)	0.1709	(2)
N	0.1331	(7)	0.6565	(10)	0.2102	(2)
O	0.1982	(6)	0.3937	(8)	0.2329	(2)
H2	0.7029	(84)	0.7500	(106)	0.0236	(21)
H3	0.4281	(89)	0.9177	(118)	0.0764	(23)
H5	0.5373	(88)	0.3393	(126)	0.2078	(22)
H6	0.8249	(83)	0.1786	(117)	0.1571	(23)
H7	0.1843	(82)	0.9036	(119)	0.1557	(23)
H8	0.0971	(85)	0.3572	(121)	0.2514	(21)

Table 2. Thermal parameters as they appear in the expression $\exp -1/4(h^2a^{*2}B_{11} + k^2b^{*2}B_{22} + l^2c^{*2}B_{33} + 2hka^*b^*B_{12} + 2hla^*c^*B_{13} + 2klb^*c^*B_{23})$.

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cl	3.93	6.96	5.11	1.08	2.13	0.49
C1	2.41	3.81	3.12	-0.51	0.54	-0.17
C2	3.82	4.23	2.56	-0.22	1.03	0.18
C3	4.12	3.67	2.75	0.23	0.22	0.44
C4	2.38	2.66	2.94	-0.32	0.11	-0.90
C5	3.16	4.61	2.48	-0.52	0.38	0.48
C6	2.55	4.97	3.17	0.40	0.31	0.64
C7	3.17	3.85	3.73	0.78	0.20	0.09
N	3.03	3.88	3.33	-0.13	0.68	-0.77
O	3.51	4.15	5.06	-0.11	2.22	0.24

Table 3. Interatomic distances and standard deviations.

Atoms	Distances (Å)	Atoms	Distances (Å)
Cl—C1	1.736 (6)	C7—N	1.284 (7)
C1—C2	1.374 (8)	N—O	1.395 (6)
C2—C3	1.384 (8)	C2—H2	1.058 (50)
C3—C4	1.399 (7)	C3—H3	0.961 (55)
C4—C5	1.393 (7)	C5—H5	1.003 (52)
C5—C6	1.368 (8)	C6—H6	0.990 (54)
C6—C1	1.378 (8)	C7—H7	0.900 (55)
C4—C7	1.465 (7)	O—H8	0.807 (54)

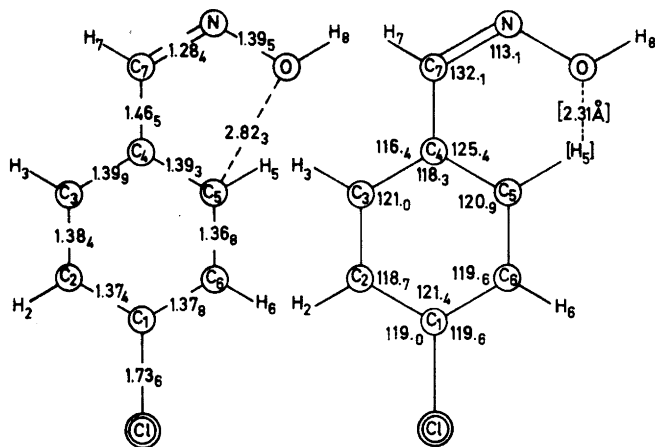


Fig. 1. Interatomic distances and angles for *anti-p*-chlorobenzaldoxime.

Table 4. Bond angles and standard deviations.

Atoms	Angles (degrees)	Atoms	Angles (degrees)
Cl—C1—C2	119.0 (0.4)	C1—C2—H2	123 (3)
Cl—C1—C6	119.6 (0.4)	C3—C2—H2	118 (3)
C6—C1—C2	121.4 (0.5)	C2—C3—H3	116 (3)
C1—C2—C3	118.7 (0.5)	C4—C3—H3	121 (3)
C2—C3—C4	121.0 (0.5)	C4—C5—H5	123 (3)
C3—C4—C5	118.3 (0.5)	C6—C5—H5	116 (3)
C4—C5—C6	120.9 (0.5)	C5—C6—H6	123 (3)
C5—C6—C1	119.6 (0.5)	C1—C6—H6	118 (3)
C3—C4—C7	116.4 (0.5)	C4—C7—H7	122 (4)
C5—C4—C7	125.4 (0.5)	N—C7—H7	105 (4)
C4—C7—N	132.1 (0.5)	N—O—H8	98 (4)
C7—N—O	113.1 (0.4)		

Table 5. Distances (in Å) from the least squares plane through Cl, C1—C6.

Atom	Deviation (Å)	Atom	Deviation (Å)
Cl	0.014	N	0.346
C1	0.001	O	0.754
C2	-0.018	H2	-0.058
C3	0.006	H3	-0.186
C4	0.010	H5	-0.007
C5	0.003	H6	0.031
C6	-0.015	H7	-0.094
C7	0.008	H8	1.042

DESCRIPTION AND DISCUSSION

The intramolecular dimensions found are summarized in Fig. 1 and in Tables 3–5. The benzene carbon atoms and the atoms directly attached to the benzene ring show no significant deviation from the expected coplanarity. None of the atoms (C and Cl) are displaced more than 0.02 Å from the least-squares plane α through the benzene carbon atoms and the chlorine atom (Table 5). The side chain attached to C4 is twisted around the bond C4–C7 in such a way that the calculated plane β through C7, N, and O forms an angle of 19.5° with the α -plane. The equations for the planes α and β are:

$$\begin{aligned}\alpha: & 0.5411x + 0.7162y + 0.4408z - 5.1603 = 0; \\ \beta: & 0.5331x + 0.4881y + 0.6911z - 5.3430 = 0;\end{aligned}$$

referring to an orthogonal coordinate system in which the x , y , and z axes coincide with the corresponding crystallographic axes and in which Ångström units are used.

The bond lengths and most of the bond angles obtained agree remarkably well with corresponding values found in the crystal structure of *syn-p*-chlorobenzaldoxime (Folting *et al.*²), although the angle between the α - and β -plane for the latter structure is only 9.5°. The difference in steric strain between the two isomers, reflected by their different deviation from coplanarity, seems to have no measurable influence on the bond lengths and it may thus be inferred that these distances are characteristic for *p*-chlorobenzaldoxime. The same conclusion may be drawn from the magnitudes of most of the bond angles, with one remarkable exception, namely, the angle $\angle C-C=N$. In *anti-p*-chlorobenzaldoxime the strain between the side chain (atom O) and the benzene ring (atoms C5 and H5) is compensated for by an expansion of the $\angle C-C=N$ angle to 132°. In *syn-p*-chlorobenzaldoxime the corresponding angle is only 121°.

Table 6. Some distances and angles in the hydrogen bonding system.

Atoms	Distances	Atoms	Angles
O–H8	0.81 (5) Å	N–O–H8	98° (4)
H8···N	1.98 (5) Å	O–H8···N	164° (6)
O···N	2.768 (6) Å	N–O···N	106.9° (.3)

The short intramolecular distances O···H5 of 2.31 Å and O···C5 of 2.82 Å correspond well to those found in *anti-p*-chloro-*N*-methylbenzaldoxime of 2.21 Å (O···H) and of 2.88 Å (O···C) (Folting *et al.*²), and with those found in *anti*-furfuraldoxime of 2.55 Å (O···H) and of 2.86 Å (O···C) (Jensen and Jerslev⁵).

The molecules are linked together by O–H···N bonds as long chains along the b -direction, as has already been established by Jerslev.¹ Some distances and angles of the hydrogen bonding system are given in Table 6.

Table 7. Observed and calculated structure factors. The reflexion with the greatest discrepancy between the observed and the calculated structure factor (18.50) is omitted from the list. That is the reflexion 701, F_o 24.81, F_c 6.31, A 0.00 and B 6.31.

H	K	L	FO	FC	A	B	H	K	L	FO	FC	A	B	H	K	L	FO	FC	A	B
0	0	4	26.94	26.12	-26.12	-0.00	5	0	4	8.61	8.54	-8.54	-0.00	2	1	13	18.10	18.11	-5.01	-17.40
0	0	6	32.43	31.84	-31.84	-0.00	5	0	5	18.29	19.04	0.00	19.04	2	1	14	13.16	13.25	2.20	13.06
0	0	8	55.71	54.99	-54.99	-0.00	5	0	6	4.30	4.52	4.52	-0.00	2	1	15	3.39	3.74	-1.96	3.21
0	0	10	54.03	52.52	-52.52	0.01	5	0	7	7.69	7.99	-0.00	7.99	2	1	16	7.04	7.34	-0.45	-5.33
0	0	12	7.71	6.58	6.58	0.00	5	0	8	3.44	3.98	-3.98	-0.00	2	1	17	23.41	24.39	-2.71	24.24
0	0	14	17.51	16.76	16.76	-0.00	5	0	9	7.44	7.44	-0.00	7.44	2	1	18	3.68	4.02	2.03	3.46
0	0	16	9.26	8.71	-8.71	-0.00	5	0	10	10.98	11.14	-11.14	-0.00	2	1	19	17.99	18.93	10.66	15.64
0	0	18	13.71	13.95	13.95	-0.00	5	0	11	12.34	11.88	-0.00	-11.88	2	1	20	8.12	8.46	2.62	-8.05
0	0	20	11.32	11.54	11.54	-0.00	5	0	12	5.06	4.92	4.92	-0.00	2	1	21	7.69	8.24	1.37	-8.12
0	0	22	10.34	11.07	11.07	0.00	5	0	13	5.83	5.81	-0.00	-5.81	2	1	22	3.69	3.95	-3.91	-0.53
0	0	24	15.17	14.33	-14.33	-0.00	5	0	15	9.76	11.15	0.01	-11.15	2	1	24	4.22	4.16	3.40	-2.41
1	0	1	1.17	0.97	0.02	-0.97	5	0	17	7.28	8.37	-0.00	-8.37	2	1	27	4.62	4.97	-2.91	-4.03
1	0	2	17.56	17.30	17.30	0.19	5	0	18	18.00	18.84	-8.84	0.00	3	1	0	10.37	9.57	0.01	-9.87
1	0	3	5.73	5.69	0.31	-5.68	5	0	20	3.99	3.97	-3.97	-0.00	3	1	1	9.50	9.24	-8.22	4.24
1	0	4	59.54	60.37	60.37	0.00	5	0	22	7.41	7.31	-7.31	0.00	3	1	2	24.68	23.77	-22.39	-7.99
1	0	5	74.79	80.04	80.04	0.00	5	0	23	6.70	7.45	-0.00	7.45	3	1	3	23.36	22.63	-20.43	-9.73
1	0	6	29.60	28.88	-28.88	0.00	5	0	25	3.51	3.40	-0.00	3.40	3	1	4	26.32	24.84	-20.28	-14.35
1	0	7	22.85	21.83	-0.00	21.83	6	0	0	8.20	8.47	8.47	0.10	3	1	5	15.18	14.70	9.86	10.89
1	0	8	17.49	16.75	16.75	-0.00	6	0	2	13.53	15.22	15.22	0.00	3	1	6	14.51	14.86	-14.42	3.58
1	0	9	6.43	6.41	0.09	-6.41	6	0	4	10.80	12.01	12.01	0.00	3	1	8	5.37	5.68	-5.47	-0.24
1	0	10	10.67	19.04	-19.04	-0.00	6	0	6	18.59	16.99	-18.99	-0.00	3	1	9	22.34	21.88	21.42	3.34
1	0	11	6.31	6.25	-0.00	6.25	6	0	8	12.49	12.91	-12.91	-0.00	3	1	10	3.20	3.03	-3.24	-2.74
1	0	12	4.50	3.80	3.80	0.00	6	0	9	3.30	2.74	0.01	-2.74	3	1	11	9.82	9.15	5.47	7.33
1	0	13	33.14	33.41	-0.00	-33.41	6	0	10	3.69	3.57	-3.57	-0.00	3	1	12	7.59	7.03	5.65	4.18
1	0	14	5.73	7.51	-7.51	0.00	6	0	12	9.82	11.39	-11.39	-0.00	3	1	13	9.12	9.39	9.01	-2.63
1	0	15	22.44	22.24	-0.00	-22.24	6	0	17	5.74	5.85	-5.85	-0.00	3	1	14	18.96	19.77	16.12	-13.85
1	0	16	12.25	12.34	12.34	-0.00	6	0	17	11.25	11.62	-0.00	-11.62	3	1	15	9.73	10.07	-9.89	1.86
1	0	17	10.50	10.43	-0.00	-10.43	6	0	18	9.27	10.19	10.19	0.00	3	1	16	4.23	4.25	2.31	3.57
1	0	18	3.48	3.39	-0.39	-0.00	6	0	20	4.75	5.25	5.25	-0.00	3	1	17	8.23	8.27	-7.62	-3.20
1	0	19	2.78	2.81	0.03	2.81	6	0	21	4.32	3.43	-0.00	-3.43	3	1	18	14.56	15.17	13.03	9.77
1	0	20	4.37	4.44	-0.00	-4.44	6	0	23	5.37	6.02	-6.02	-0.00	3	1	19	7.12	7.15	-5.21	-4.86
1	0	21	6.96	7.74	-0.00	-7.74	7	0	7	12.70	13.85	0.02	13.85	3	1	20	4.49	4.95	0.24	-4.95
1	0	23	3.46	4.03	-0.00	-4.03	7	0	8	3.51	3.73	3.73	0.00	3	1	22	3.82	4.19	-3.98	-1.30
1	0	24	1.02	2.62	-2.62	-0.00	7	0	9	3.95	5.68	-0.00	-5.68	3	1	24	7.70	9.21	-8.67	3.12
1	0	25	4.35	4.12	0.00	4.12	7	0	12	7.18	6.79	-6.79	-0.00	3	1	25	4.03	4.59	6.33	5.99
1	0	27	3.43	4.57	-0.00	-4.57	7	0	13	11.92	12.64	0.00	-12.64	3	1	30	3.49	2.60	-0.07	2.60
2	0	0	12.58	11.65	11.65	0.00	7	0	15	3.81	4.03	-0.00	-4.03	4	1	0	11.38	10.87	-10.87	-0.00
2	0	1	12.58	12.56	0.05	12.56	7	0	16	4.95	4.74	-4.74	0.00	4	1	1	21.49	21.02	-5.33	-20.33
2	0	2	53.66	53.86	53.86	0.32	7	0	17	3.40	4.04	-4.04	-0.00	4	1	2	11.18	11.40	-6.52	-9.77
2	0	3	16.46	15.29	-0.00	-15.29	8	0	0	4.97	5.49	5.49	0.00	4	1	3	13.35	13.63	9.33	9.93
2	0	5	32.35	32.25	-0.05	-32.25	8	0	2	4.46	4.81	4.81	-0.00	4	1	4	18.38	18.22	12.44	-13.31
2	0	6	7.26	8.09	-8.09	-0.00	8	0	7	5.85	6.06	0.03	-6.06	4	1	5	5.88	5.79	-5.15	-2.66
2	0	7	34.46	33.64	-33.64	-0.00	8	0	8	6.05	6.34	-6.34	-0.00	4	1	7	16.18	16.14	4.58	-15.47
2	0	8	36.36	35.04	-35.04	-0.00	8	0	12	4.28	4.95	-4.95	-0.00	4	1	8	9.92	9.81	-9.92	1.17
2	0	9	4.21	3.72	0.00	3.72	9	0	5	4.20	4.11	-0.00	4.11	4	1	9	16.59	16.32	-12.08	-10.97
2	0	10	16.26	16.23	-0.00	-16.23	9	0	1	33.41	33.38	-0.00	33.38	4	1	10	3.36	3.34	0.77	3.25
2	0	11	2.48	2.51	-0.03	-0.03	9	0	4	2.93	2.82	0.68	-2.74	4	1	11	25.49	26.65	-0.58	-26.65
2	0	12	20.99	20.35	-20.35	-0.00	9	0	5	2.38	2.10	0.00	-2.10	4	1	12	6.41	6.93	-6.86	-5.72
2	0	13	7.20	7.35	-0.00	-7.35	0	1	6	32.00	31.06	0.02	-31.06	4	1	13	9.41	10.01	9.03	-4.32
2	0	14	4.32	4.43	-0.43	-0.00	0	1	7	5.29	4.89	0.55	-4.86	4	1	14	9.20	8.75	-8.74	0.25
2	0	15	0.04	4.24	-4.24	0.00	0	1	8	4.92	5.08	0.05	-5.08	4	1	15	13.57	13.66	-1.93	13.53
2	0	16	5.83	5.73	-0.00	-5.73	0	1	9	20.21	30.57	-0.00	-30.57	4	1	16	4.35	4.47	-2.16	2.72
2	0	17	12.23	12.20	-0.00	-12.20	0	1	11	36.41	36.53	0.09	-36.53	4	1	17	3.83	4.70	-1.16	1.76
2	0	18	11.97	12.75	12.75	-0.00	0	1	12	28.44	28.00	-0.00	28.00	4	1	19	8.59	9.93	1.79	9.76
2	0	19	5.78	5.07	-0.00	-5.07	0	1	13	7.37	5.85	-0.00	-5.85	4	1	20	3.88	4.85	-0.02	4.85
2	0	20	15.10	15.22	0.00	0.00	0	1	14	5.51	5.13	0.03	-5.12	4	1	21	6.17	6.37	-0.64	6.33
2	0	21	10.72	11.37	-0.00	-11.37	0	1	16	4.04	4.49	0.07	-4.49	4	1	22	6.30	6.45	-6.02	-5.33
2	0	22	3.69	3.17	-0.00	-3.17	0	1	17	16.40	17.13	-0.00	-17.13	4	1	25	6.22	6.09	5.42	-2.78
2	0	25	4.17	4.06	-0.00	-4.06	0	1	19	3.57	3.54	0.00	3.54	4	1	26	4.57	4.73	3.99	-2.54
2	0	27	4.03	4.19	-0.49	-0.00	0	1	21	10.85	11.95	0.00	11.95	5	1	0	4.95	5.39	-0.00	5.33
2	0	29	4.03	4.09	-0.00	-4.09	0	1	22	4.05	4.05	0.00	4.05	5	1	1	13.85	13.98	-10.13	-9.44
3	0	1	28.16	26.13	-0.00	-26.13	0	1	24	6.42	6.26	0.00	-6.26	5	1	2	14.88	16.89	-6.45	-6.02
3	0	2	17.82	16.87	-16.87	0.10	0	1	28	3.33	3.41	-0.00	-3.41	5	1	3	8.48	9.88	-0.54	9.87
3	0	3	44.19	43.52	0.00	43.52	0	1	31	3.79	1.63	0.00	-1.63	5	1	4	16.55	16.44	-16.44	-0.11
3	0	4	16.04	15.79	-0.00	-15.79	0	1	32	4.07	2.78	0.00	-2.78	5	1	5	8.74	9.31	1.49	-9.19
3	0	5	31.84	28.93	0.00	28.93	1	1	0	9.16	8.88	0.01	8.88	5	1	6	19.04	20.02	-19.67	3.72
3	0	6	17.54	16.09	16.09	-0.00	1	1	1	34.77	32.83	-7.54	31.95	5	1	7	10.07	10.49	6.87	7.93
3	0	7	37.85	37.30	0.00	37.30	1	1	2	61.25	61.49	-50.97	34.40	5	1	8	5.26	4.68	4.57	-1.04
3	0	8	13.66	12.84	12.84	0.08	1	1	3	29.28	27.78	-26.75	7.47	5	1	9	7.28	8.19	3.00	7.42
3	0	9	10.74	11.18	-0.00	-11.18	1	1	4	76.19										

Table 7. Continued.

H	K	L	FO	FC	A	B	H	K	L	FO	FC	A	B	H	K	L	FO	FC	A	B	
7	1	8	4.49	5.38	-5.16	-1.52	4	2	3	10.33	10.34	10.24	-1.43	2	3	1	10.31	10.78	-9.36	-5.34	
7	1	9	5.75	6.19	5.42	2.98	4	2	4	6.00	5.73	4.21	3.89	2	3	2	9.51	9.50	5.77	7.55	
7	1	10	4.82	4.81	4.40	1.94	4	2	5	14.25	14.16	14.55	-2.47	2	3	3	3.31	3.70	2.90	2.73	
7	1	11	5.42	6.39	4.95	4.04	4	2	7	5.02	6.00	6.89	-0.31	2	3	4	15.82	15.41	-2.12	15.27	
7	1	14	6.32	7.00	6.18	-3.29	4	2	8	8.99	9.48	7.89	5.25	2	3	5	11.66	11.37	-10.39	-4.63	
7	1	16	4.66	5.48	5.48	0.12	4	2	9	3.33	3.94	2.02	-3.39	2	3	6	10.62	10.28	-4.50	9.24	
7	1	19	5.65	6.94	-4.25	-5.49	4	2	10	14.69	15.49	9.20	-12.47	2	3	8	5.09	4.77	-1.19	4.62	
8	1	4	4.50	5.04	0.64	4.36	4	2	11	5.04	5.59	-5.38	1.52	2	3	9	8.27	8.27	7.84	2.64	
8	1	3	6.08	5.63	3.75	4.21	4	2	12	3.13	3.07	0.45	-3.03	2	3	10	7.60	7.64	6.12	-4.58	
8	1	9	6.47	7.41	-4.36	-5.99	4	2	13	12.55	13.18	-13.15	-0.79	2	3	11	6.04	6.31	-0.38	6.30	
8	1	11	6.07	7.31	-0.63	-7.28	4	2	14	4.19	3.91	3.67	-1.34	2	3	12	3.13	3.21	-1.34	-2.92	
8	1	15	5.38	5.62	1.89	5.29	4	2	15	4.33	4.13	-3.51	-2.17	2	3	13	6.73	6.56	5.84	-2.97	
9	1	4	4.38	5.04	-4.15	2.86	4	2	16	5.34	5.36	-1.38	5.18	2	3	14	6.93	7.14	1.53	-6.98	
0	2	3	9.70	9.92	9.92	0.37	4	2	17	3.72	3.86	-2.75	-2.71	2	3	16	4.58	4.27	0.63	-4.23	
0	2	4	4.85	4.07	4.07	-0.00	4	2	18	4.43	5.26	-5.20	-0.74	2	3	18	4.59	4.99	-2.18	-4.48	
0	2	5	22.99	22.70	22.70	0.00	4	2	20	5.36	6.10	-2.37	5.62	2	3	19	4.28	4.56	-4.47	0.90	
0	2	8	19.47	17.87	17.87	0.11	4	2	22	3.73	4.90	-4.88	0.47	2	3	21	3.97	4.23	-3.36	-2.56	
0	2	9	10.23	9.63	9.63	0.20	4	2	23	4.82	5.84	4.09	4.17	3	3	0	8.88	9.21	0.00	9.21	
0	2	10	12.74	12.67	12.67	0.06	4	2	25	3.53	3.97	3.97	-0.06	3	3	1	18.27	18.13	14.76	10.54	
0	2	11	15.92	16.43	-16.43	-0.00	4	2	26	3.54	3.79	3.01	-2.31	3	3	2	10.40	9.98	9.07	-4.16	
0	2	12	11.38	11.07	11.07	-0.00	5	2	0	18.70	19.68	0.00	-19.68	3	3	3	14.14	14.37	12.12	-8.09	
0	2	13	7.50	8.03	8.03	-0.00	5	2	1	8.42	8.65	-7.40	4.48	3	3	4	9.69	9.72	7.02	-6.73	
0	2	14	2.71	2.87	-2.87	-0.00	5	2	2	6.27	6.79	5.83	-3.48	3	3	5	11.90	11.93	-0.58	-8.28	
0	2	15	13.37	13.19	-13.19	0.00	5	2	3	5.93	6.82	6.52	-2.00	3	3	6	7.15	7.84	4.40	6.49	
0	2	17	7.56	7.58	-7.58	-0.00	5	2	4	7.73	8.13	-1.88	-7.9	3	3	7	7.57	8.26	-6.36	5.30	
0	2	18	4.72	4.49	-4.49	-0.00	5	2	5	5.16	5.90	2.47	-5.36	3	3	8	6.87	7.35	-7.26	1.12	
0	2	20	6.01	7.23	-7.23	0.00	5	2	6	10.55	11.86	-1.05	11.81	3	3	9	16.55	17.40	-16.86	4.29	
0	2	21	4.95	4.71	-4.71	0.00	5	2	7	12.12	12.90	-9.33	-8.91	3	3	10	7.59	4.34	-1.95	-3.87	
0	2	23	4.68	5.94	5.94	0.00	5	2	8	10.33	10.00	-0.34	10.05	3	3	11	7.93	8.12	-4.95	-6.41	
0	2	25	3.31	3.11	-3.11	-0.00	5	2	9	7.36	8.35	6.05	-0.75	3	3	12	4.98	5.73	-2.88	3.76	
0	2	26	4.87	5.39	5.39	0.00	5	2	10	10.87	10.78	-9.47	5.16	3	3	14	9.01	9.63	4.53	8.50	
0	2	27	5.11	5.05	5.05	0.00	5	2	11	3.78	4.54	3.84	2.44	3	3	15	2.77	3.77	3.45	-1.52	
1	2	0	29.11	28.60	0.00	-28.60	5	2	13	8.99	9.95	-3.91	9.15	3	3	16	3.65	3.85	-3.76	0.85	
1	2	1	8.10	7.43	-7.43	-0.13	5	2	14	6.55	5.36	5.31	-7.3	3	3	17	7.03	8.22	-1.60	-1.60	
1	2	2	29.09	28.56	10.82	-26.44	5	2	15	6.71	8.04	1.64	7.88	3	3	19	6.06	6.49	3.98	5.13	
1	2	3	18.46	17.97	17.97	0.05	5	2	16	3.15	2.89	-2.13	-1.94	3	3	21	3.46	3.19	3.18	0.12	
1	2	4	9.61	8.07	-8.07	-0.18	5	2	17	3.43	3.67	-2.93	2.22	3	3	24	3.43	3.86	2.59	-2.87	
1	2	5	15.24	15.74	15.74	-0.16	5	2	18	7.44	6.77	-7.44	7.83	3	3	27	7.83	7.83	-7.83	-7.83	
1	2	6	17.67	17.30	2.16	-17.17	5	2	21	4.48	5.44	-3.79	-3.91	4	3	0	5.94	7.13	-7.13	0.00	
1	2	7	29.86	28.39	-14.39	-24.47	6	2	0	5.77	6.57	-6.57	0.00	4	3	1	9.50	9.73	8.84	4.06	
1	2	8	8.81	8.62	-4.33	7.45	6	2	2	9.73	9.88	-9.07	5.86	4	3	2	5.99	6.44	-4.36	4.75	
1	2	9	6.96	6.78	-1.32	-6.65	6	2	3	4.13	3.09	3.06	-0.43	4	3	3	5.89	6.17	2.63	5.58	
1	2	10	31.52	30.39	-13.09	-27.43	6	2	4	11.43	11.40	-11.43	0.00	4	3	4	11.33	11.33	11.33	11.33	
1	2	11	7.88	7.33	-5.02	5.34	6	2	5	7.77	7.90	6.11	5.00	4	3	6	5.25	5.25	-5.01	1.59	
1	2	12	11.67	11.67	9.32	7.03	6	2	6	7.60	8.67	8.24	2.72	4	3	8	10.47	11.14	5.54	9.66	
1	2	13	12.94	12.50	3.79	11.91	6	2	8	6.62	6.55	6.55	0.06	4	3	9	3.44	4.10	3.79	1.57	
1	2	14	8.03	7.93	-0.55	0.93	6	2	9	3.24	3.09	2.64	-1.60	4	3	10	2.94	2.41	-2.41	0.00	
1	2	15	12.90	13.48	-3.50	13.02	6	2	10	7.85	3.37	1.47	3.03	4	3	11	6.34	7.13	-2.26	6.76	
1	2	16	8.13	8.43	-2.15	-8.15	6	2	11	3.18	2.74	0.64	-2.66	4	3	12	7.31	7.22	-2.23	-6.87	
1	2	17	17.17	18.02	17.00	5.96	6	2	12	8.21	8.57	1.25	-8.48	4	3	13	3.83	4.57	-2.04	4.08	
1	2	18	3.34	3.45	-1.55	-3.68	6	2	13	5.02	5.46	-4.75	-2.91	4	3	15	5.09	5.09	-0.05	-5.09	
1	2	19	8.84	8.10	-6.10	-3.27	-1.43	6	2	14	3.33	4.01	-3.81	-1.24	4	3	16	5.37	5.82	-7.10	-4.93
1	2	20	8.91	8.99	1.40	-3.08	6	2	23	3.59	3.99	3.78	1.28	4	3	18	4.23	4.94	1.73	-3.63	
1	2	21	3.92	5.01	-1.73	-4.70	7	2	1	3.80	4.02	2.86	-2.83	4	3	22	3.85	4.59	-0.11	4.59	
1	2	22	7.70	7.65	-5.44	-5.37	7	2	2	6.24	7.04	-1.41	-6.90	4	3	26	4.11	1.85	1.83	0.31	
1	2	23	3.27	3.27	0.76	0.76	7	2	3	3.87	3.54	-3.54	3.54	4	3	3	5.45	5.3	-4.6	0.70	
1	2	24	7.27	8.34	2.65	7.90	7	2	5	4.46	4.15	-0.04	-4.15	5	3	2	3.45	4.41	-0.23	4.40	
1	2	26	3.79	3.24	3.24	-0.06	7	2	7	4.18	4.84	-4.70	-1.16	5	3	3	4.15	4.06	4.02	0.61	
1	2	30	3.46	2.58	0.09	2.58	7	2	8	7.23	7.12	-1.75	6.90	5	3	4	4.83	4.69	3.48	-3.14	
1	2	31	4.12	3.66	3.62	-1.27	7	2	10	5.20	5.36	2.46	-3.33	5	3	5	2.66	3.38	0.75	-3.29	
2	2	0	17.46	16.46	-16.46	0.13	7	2	9	5.76	5.63	3.31	4.56	5	3	6	3.36	3.48	-3.48	-3.38	
2	2	1	10.44	10.22	-10.05	-1.82	7	2	15	4.82	4.06	3.88	1.20	3	3	8	3.65	3.92	2.90	-2.63	
2	2	2	23.68	23.05	-22.85	3.03	7	2	16	4.59	4.95	2.68	-4.16	3	3	9	5.68	6.65	-6.65	0.13	
2	2	3	18.69	18.49	18.35	-2.23	7	2	18	6.14	5.69	0.61	-5.66	5	3	10	3.00	3.58	-1.51	-3.24	
2	2	4	12.90	12.20	-12.20	-0.26	7	2	19	4.40	4.12	-4.12	1.64	5	3	11	11.12	11.14	-7.03	-4.06	
2	2	5	23.49	22.42	-22.29	-2.41	8	2	0	6.44	7.45	-7.45	0.02	5	3	12	4.85	5.41	1.16	5.29	
2	2	6	35.14	33.96	31.70	-12.17	8	2	3	5.49	6.53	6.52	0.28	5	3	14	3.50	3.55	-3.40	1.00	
2	2	7	27.64	26.36	-25.32	-7.34	8	2	9	4.19	4.08	4.08	0.16	5	3	16	4.47	4.46	1.28	4.27	
2	2	8	18.63	13.20	6.77	13.34	8	2	13	5.53	6.42	-4.41	-4.32	5	3	17	3.61	5.54	-5.53	3.29	
2	2	9	12.08	11.69	-11.15	-3.51	0	3	1	13.12	13.39	-0.00	-13.39	5	3	18	2.69	2.69	-2.62	0.63	
2	2	10	2.51	2.08	-0.05	2.08	0	3	4	6.79	7.67	0.00	7.67	5	3	19	3.63	3.18	3		

Table 7. Continued.

H	K	L	FD	FC	A	B	H	K	L	FD	FC	A	B	H	K	L	FD	FC	A	B
1	4	0	7.54	7.44	0.00	9.44	2	4	7	7.96	8.61	-1.03	8.54	4	4	0	5.02	5.10	5.10	0.04
1	4	1	2.26	2.73	-2.53	-1.40	2	4	8	3.48	3.24	3.24	-0.04	4	4	1	4.95	4.64	-4.32	1.68
1	4	2	7.10	8.46	-1.97	8.23	2	4	9	2.65	3.22	2.84	-1.53	4	4	3	4.93	5.07	-3.27	-3.87
1	4	3	5.48	3.57	-3.52	0.60	2	4	10	2.98	3.36	3.33	-0.27	4	4	5	3.86	3.52	-3.39	0.94
1	4	4	1.64	1.42	-1.04	-0.97	2	4	11	2.85	2.85	2.31	1.66	4	4	7	5.58	5.95	-5.91	0.63
1	4	5	8.08	8.92	5.15	-7.28	2	4	13	3.15	2.70	7.58	-0.81	4	4	8	3.41	4.06	-3.67	1.74
1	4	6	2.78	2.92	2.85	-0.64	2	4	15	3.84	3.36	3.34	0.32	4	4	10	4.67	4.70	4.36	-1.73
1	4	7	4.33	4.91	3.15	-3.76	2	4	16	3.19	2.61	-1.03	-2.40	4	4	11	3.73	4.18	0.78	-4.11
1	4	8	9.78	9.78	-6.69	-7.13	2	4	17	3.82	3.82	2.59	-2.81	4	4	12	3.86	4.19	2.15	3.60
1	4	9	7.08	7.35	4.04	6.15	2	4	18	3.43	1.84	-1.83	0.20	4	4	13	8.20	8.75	7.76	4.05
1	4	10	11.74	12.29	7.68	-9.40	2	4	21	3.40	3.28	-2.10	2.52	4	4	15	3.21	2.91	2.83	0.60
1	4	11	7.15	7.96	-7.15	-3.49	3	4	0	11.80	12.54	0.00	12.54	4	4	16	3.26	3.11	-2.60	-1.35
1	4	12	2.91	2.58	-2.39	-0.96	3	4	1	3.48	3.33	1.11	3.12	4	4	24	3.77	2.29	2.07	0.97
1	4	13	2.28	2.52	-0.94	-2.34	3	4	2	6.46	6.61	6.53	1.05	5	4	2	4.15	4.27	0.55	4.23
1	4	16	3.22	4.10	1.23	3.91	3	4	3	8.96	9.18	2.17	-8.92	5	4	4	6.03	5.98	5.11	3.11
1	4	18	3.94	4.42	-1.42	4.18	3	4	4	3.75	3.91	-3.80	0.92	5	4	8	4.97	4.98	1.68	-4.68
1	4	20	3.49	2.28	-2.10	0.89	3	4	5	2.98	2.57	-1.57	-2.04	5	4	11	3.68	3.82	-3.58	1.34
1	4	21	3.09	2.30	1.60	1.65	3	4	6	2.52	2.68	-1.02	-2.47	5	4	12	4.53	5.43	-2.85	-4.62
1	4	28	3.23	1.56	1.41	-0.66	3	4	7	3.37	3.80	-3.77	-0.53	6	4	4	4.42	3.29	-2.85	-1.63
2	4	1	3.25	3.40	-2.23	-2.57	3	4	8	6.62	6.92	5.53	-4.16	6	4	10	3.15	0.34	-0.27	0.21
2	4	3	5.88	6.58	-6.58	-0.11	3	4	9	4.57	5.23	3.12	4.19	6	4	15	3.02	3.01	2.64	1.45
2	4	4	5.37	5.18	3.53	-3.79	3	4	10	2.75	3.27	-1.05	-3.10	7	4	6	3.33	3.28	0.16	-3.27
2	4	5	14.07	14.52	-14.14	-3.27	3	4	12	3.88	3.74	-3.06	-2.14	7	4	10	3.59	2.13	0.30	-2.11
2	4	6	10.44	11.06	-9.00	6.43	3	4	20	3.26	2.43	0.99	2.22	7	4	15	3.86	3.10	-1.78	-2.53
														8	4	4	4.09	2.08	-1.77	1.09

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