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The Crystal Structure of Copper Dimethylglyoxime Dichloride

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The crystal structure of copper dimethylglyoxime dichloride, $Cu(C_4H_8O_2N_2)Cl_2$, has been determined by three-dimensional X-ray methods. The space group of the structure is $P\bar{1}$ and the unit cell dimensions are $a=7.697$ Å, $b=8.174$ Å, $c=8.120$ Å, $\alpha=108.13°$, $\beta=69.16°$, and $\gamma=78.69°$.

The structure can be visualised as being built up from two parallel coplanar copper dimethylglyoxime chains facing one another and held together by two chlorine bridges between the copper atoms. The copper atom is thus five-coordinated by a distorted square planar arrangement of two nitrogen atoms and two chlorine atoms within the same molecule, and a chlorine atom belonging primarily to the adjacent molecule. The presence of two hydrogen bonds was indicated by the infrared spectrum of the salt. One of them probably links the copper dimethylglyoxime dichloride molecules together to form the chain and the other is probably an intramolecular hydrogen bond of the type $O-H\cdots Cl$.

The aim of this work was to contribute to a research programme already in progress at this Department concerning the coordination chemistry of the transition metals and to clarify a problem connected with studies of the properties of metal dioximes at the Department of Analytical Chemistry.

Since the reaction between nickel(II) and dimethylglyoxime was first reported by Tchugaeff[1] in 1905, many attempts have been made to elucidate the selective properties of dimethylglyoxime for certain metal ions. Ni(II), Cu(II), Pd(II), and Pt(II) have been found to form complexes with the composition $M(HD)_2$, where H_2D is the acid form of the dioxime. Composite salts have also been synthesised. Paneth and Thilo[2] prepared $Ni(H_2D)_2Cl_2$, Feigl and Rubenstein[3] both $Co(H_2D)Cl_2$ and $Co(H_2D)_2Br_2$, and Dubsky and Brychta[4] $Ni(H_2D)_2Br_2$. Thilo[5] was the first to report the existence of the compound, $Cu(H_2D)Cl_2$. The coordination chemistry of the dioximes has been reviewed by Dyrssen.[6]

THE COMPOUND

Copper dimethylglyoxime dichloride was prepared by Ivanova using the method of Cox *et al.*[7] Cold alcoholic solutions of anhydrous copper(II) chloride (15 mmoles in 80 ml ethanol) and dimethylglyoxime (17 mmoles in 120 ml ethanol) were mixed together, whereupon deep green, plate-shaped crystals rapidly separated. The product was washed with absolute ethanol and dried. It was found to be stable in air but it decomposed in water probably by disproportionation:

$$2Cu(H_2D)Cl_2 \rightleftharpoons Cu(HD)_2 + Cu^{2+} + 2H^+ + 4Cl^-$$

A chemical analysis yielded the following results:

	% C	% H	% N	% Cu	% Cl
Experimental	19.52	3.22	11.28	24.9	28.4
Theoretical	19.17	3.22	11.18	25.3	28.3

The compound undergoes a violent exothermal decomposition when heated to 215°C in argon atmosphere, and thereby loses 35.9 ± 0.1 % of its original weight. An X-ray powder investigation of the residue showed that it contained, besides carbon, copper(I) chloride. The decomposition reaction was studied using a Mettler recording vacuum thermo-analyzer.

THE INFRARED SPECTRUM

The IR spectrum of dimethylglyoxime and the copper complexes $Cu(HD)_2$ and $Cu(H_2D)Cl_2$ in the solid state were recorded on a Beckman spectrophotometer, model IR9, using the potassium bromide disc technique. In the region 3200—3340 cm^{-1} two separate absorption peaks were observed for $Cu(H_2D)Cl_2$ at 3220 cm^{-1} and 3310 cm^{-1}, respectively. This is the region where the effects of hydrogen bonding on the O—H stretching frequency are to be expected. The absorption at 3310 cm^{-1} is in good agreement with a polymeric intermolecular O—H···O association as found by Nakamoto *et al.*[8] According to the estimations by Nakamoto an absorption at 3310 cm^{-1} corresponds to an oxygen-oxygen distance of 2.80 Å (found 2.90 Å). The absorption peak at 3220 cm^{-1} is probably due to an intramolecular hydrogen bond of the type O—H···Cl. Oximes[9,10] normally show an absorption band in the region 1600—1700 cm^{-1} due to C=N stretching vibrations. This band is, however, displaced to lower frequencies in the spectra of $Cu(HD)_2$ and $Cu(H_2D)Cl_2$ in which the oxime groups are linked to the copper atom by nitrogen-metal bonds. The shift is most likely due to a displacement of electron charge from the double bond to the region between the copper and the nitrogen atom. It is difficult to explain why the shift is larger for $Cu(H_2D)Cl_2$ than for $Cu(HD)_2$ since the Cu—N bond lengths are practically equal. Fig. 1 shows a comparison of the IR spectra of the related compounds.

STRUCTURE DETERMINATION

The layers $0kl$ to $\bar{6}kl$ (989 reflections) and $h0l$ to $h6l$ (792 reflections) were registered according to the single crystal Weissenberg method using multiple film techniques and $CuK\alpha$-radiation. The relative intensities of the reflections were estimated visually by comparison with a standard scale. The structure was found to be triclinic. From the zerolayer photographs ($0kl$,

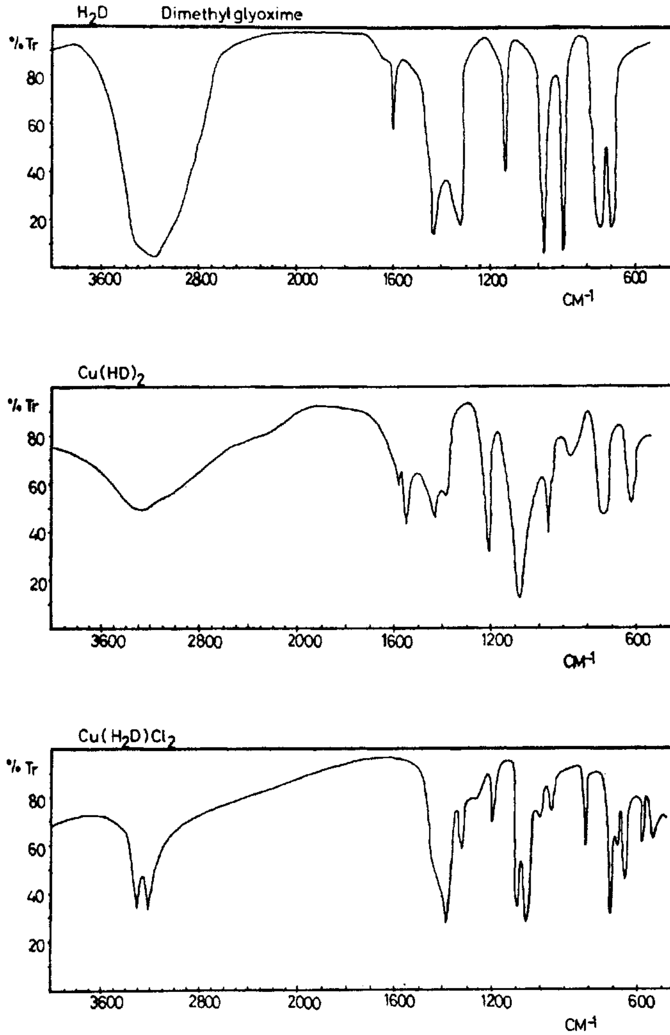

Fig. 1. The IR spectra (KBr) of dimethylglyoxime, copper bisdimethylglyoxime and copper dimethylglyoxime dichloride.

h0l, and *hk*0) it was then possible to choose and to approximately estimate the cell constants.

Accurate cell dimensions were determined from Guinier powder photographs, using $Pb(NO_3)_2$ as internal standard and $CuK\alpha_1$ radiation ($\lambda(CuK\alpha_1)=1.54050$ Å). 74 reflections were indexed with the computer pro-

Table 1. Powder data.

h	k	l	$\sin^2\theta$(obs.) $\times 10^6$	$\sin^2\theta$(calc.) $\times 10^6$	I(Guinier) obs.	I(Weiss.) obs.
0	1	0	11 166	11 163	vs	122
−1	0	0	12 983	13 018	vs	—
0	−1	1	13 788	13 813	m	30
−1	−1	0	15 812	15 853	vs	—
−1	1	−1	23 748	23 771	m	28
−1	1	0	32 440	32 511	vw	9
0	1	1	33 444	33 421	m	36
−1	0	1	36 896	36 861	m	36
0	2	−1	37 440	37 499	w	72
−1	1	−2	40 019	39 938	m+	47
0	1	−2	41 327	41 370	m+	51
−1	−2	1	45 215	45 250	vw	5
−2	0	0	52 090	52 074	s	61
0	−2	2	55 299	55 252	vs	290
−2	0	−2	56 331	56 331	w	26
−2	1	−1	59 806	59 766	w	36
−1	−1	−2	62 529	62 496	m	66
−2	−2	0	63 439	63 413	vw	43
−2	−1	−2	70 394	70 444	m	61
−2	−2	−1	72 678	72 695	m−	33
−1	−2	2	74 405	74 392	m	145
−2	1	0	79 900	79 895	s	145
−1	0	2	85 713	85 612	w	15
−2	0	1	87 327	87 307	vw	30
−1	−3	0	88 458	88 503	vw	22
0	−3	2	91 350	91 462	m	86
0	1	−3	93 846	93 834	w	18
−3	0	−1	95 490	95 452	s	61
0	−2	3	97 925	97 912	w	18
−1	−3	2	102 156	102 273	m	43
−3	−1	0	103 293	103 344	m	79
−1	−2	−2	107 354	107 266	s	145
−3	−2	0	112 033	111 848	w	30
−3	0	0	117 242	117 167	m+	145
−2	−2	2	119 661	119 570	w	24
−2	−1	2	122 470	122 345	m	51
−1	−1	−3	123 166	123 179	w	28
0	3	−3	124 235	124 312	vw	24
−3	0	−3	126 674	126 744	vw	18
−1	3	−3	128 339	128 154	w	10
−2	2	0	129 971	130 044	m	43
−3	−2	−2	132 541	132 542	w	43
0	2	2	133 601	133 685	w	17
−3	−2	1	139 039	138 863	vw	28
−3	−1	−3	142 337	142 333	vw	18
−1	1	−4	146 902	146 995	w	15
−2	0	2	147 389	147 447	m−	30
−2	1	−4	148 674	148 822	m	26
−2	3	−3	158 027	158 028	w	43
−2	0	−4	160 219	160 217	w+	26
−3	2	−3	162 699	162 547	w+	43
−4	−1	−2	164 453	164 452	m	26
−1	0	−4	166 773	166 719	m+	36
−4	−2	−1	172 866	172 825	w+	30
−4	−2	0	186 231	186 321	m	36

Table 1. Continued.

−4 −1 −3	191 067	190 966	m+	61
−3 −1 2	202 032	201 888	w	43
−4 −3 0	208 639	208 823	w	51
−3 3 −2	215 275	215 252	w−	36
−4 −2 −3	220 534	220 554	m+	72
−2 1 −5	228 446	228 322	vw	13
−1 1 −5	237 805	237 885	w+	36
−3 1 −5	244 754	244 796	vw	15
−5 −1 −2	250 580	250 512	vw	9
−3 2 −5	254 325	254 253	vw	11
−2 2 2	264 680	264 633	vw	15
−5 −2 −2	261 983	261 967	w	30
−3 −2 3	267 553	267 613	vw	15
−1 3 2	269 825	269 895	vw	30
0 5 0	279 198	279 087	vvw	3
−4 1 −5	287 199	287 307	w+	36
−5 0 −4	297 038	296 933	vw	18
−1 1 4	316 596	316 544	vw	9
−5 1 −1	323 778	323 975	vw	18

w = weak; vw = very weak; m = medium; s = strong; vs = very strong.

Table 2. Atomic co-ordinates, expressed as fractions of the cell edges, and isotropic thermal parameters in Å² for copper dimethylglyoxime dichloride.

Atom	$x \pm \sigma(x)$	$y \pm \sigma(y)$	$z \pm \sigma(z)$	$B \pm \sigma(B)$
Cu	0.00084 ± 0.00024	0.00808 ± 0.00024	0.71420 ± 0.00024	3.49 ± 0.05
Cl1	0.96345 ± 0.00047	0.79022 ± 0.00047	0.49528 ± 0.00045	3.25 ± 0.07
Cl2	0.32787 ± 0.00048	0.88040 ± 0.00048	0.61194 ± 0.00046	3.37 ± 0.07
O1	0.13568 ± 0.00150	0.22878 ± 0.00157	0.98257 ± 0.00158	4.45 ± 0.21
O2	0.56335 ± 0.00153	0.09175 ± 0.00151	0.82163 ± 0.00155	4.34 ± 0.20
N1	0.97923 ± 0.00154	0.19428 ± 0.00154	0.94827 ± 0.00151	3.04 ± 0.19
N2	0.70671 ± 0.00161	0.14227 ± 0.00164	0.87023 ± 0.00162	3.43 ± 0.21
C1	0.80702 ± 0.00173	0.31311 ± 0.00181	0.08011 ± 0.00173	2.90 ± 0.22
C2	0.64619 ± 0.00189	0.27667 ± 0.00193	0.03011 ± 0.00186	3.07 ± 0.23
C3	0.77311 ± 0.00234	0.47801 ± 0.00240	0.25362 ± 0.00232	4.52 ± 0.30
C4	0.43001 ± 0.00215	0.38682 ± 0.00221	0.17322 ± 0.00213	4.03 ± 0.28

gramme Powder [11] and the same programme was used to refine the cell constants. The unit cell dimensions were found to be:

$a = 7.6970 \pm 0.0006$ Å
$b = 8.1743 \pm 0.0012$ Å
$c = 8.1203 \pm 0.0007$ Å
$\alpha = 108.135 \pm 0.009°$
$\beta = 69.160 \pm 0.006°$
$\gamma = 78.692 \pm 0.008°$
$V = 425.84$ Å³

Observed and calculated values of $\sin^2\theta$ and the corresponding intensities of the reflections are listed in Table 1. The density was determined to be 1.95 g/cm³, indicating two formula units per unit cell (calculated density = 1.96 g/cm³).

A three-dimensional Patterson synthesis based on the data from the a-axis indicated that the space group of the structure was $P\bar{1}$ and revealed the parameters of the copper and chlorine atoms. Using the signs of the structure factors obtained with these positions a three dimensional Fourier calculation was performed from which the positions of the light atoms could be determined. After a few cycles of isotropic least squares refinement the R-value converged to 0.158. At this stage the data from the b-axis was available and in order to obtain improved standard deviations of the atomic parameters

Table 3. Interatomic distances and angles with their standard deviations.

Bond	$L \pm \sigma$ (Å)	Angle	$\theta \pm \sigma°$
Cu–Cu′	3.445 ± 0.003	Cl1′–Cu –N1	96.79 ± 0.33
Cu–N1	1.958 ± 0.011	Cl1′–Cu –O1	94.20 ± 0.23
Cu–N2	2.013 ± 0.011	Cl1′–Cu –N2	92.29 ± 0.34
Cu–Cl1	2.238 ± 0.004	Cl1′–Cu –O2	92.07 ± 0.22
Cu–Cl2	2.249 ± 0.004	Cl1′–Cu –Cl1	92.00 ± 0.13
Cu–Cl1′	2.698 ± 0.004	Cl1′–Cu –Cl2	95.58 ± 0.12
Cu–O1	2.996 ± 0.011	Cl2 –Cu –Cl1	98.62 ± 0.14
Cu–O2	3.034 ± 0.010	Cl2 –Cu –N1	90.50 ± 0.32
O1–N1	1.389 ± 0.015	Cl2 –Cu –N2	165.93 ± 0.34
O1–O2	2.895 ± 0.014	Cl1 –Cu –N1	166.68 ± 0.33
O1–Cl2	3.033 ± 0.012	Cl1 –Cu –N2	92.73 ± 0.34
O2–N2	1.390 ± 0.015	N1 –Cu –N2	76.98 ± 0.45
O2–Cl1	3.120 ± 0.011	Cu –Cl1–Cu′	88.00 ± 0.13
N1–C1	1.298 ± 0.016	Cu –N1 –O1	126.23 ± 0.80
N2–C2	1.271 ± 0.018	Cu –N2 –O2	125.11 ± 0.85
C1–C2	1.480 ± 0.018	Cu –N1 –C1	119.86 ± 0.86
C1–C3	1.513 ± 0.018	Cu –N2 –C2	117.62 ± 0.91
O2–Cl2	3.281 ± 0.011	N1 –O1 –O2	142.25 ± 0.81
C2–C4	1.519 ± 0.020	N2 –O2 –O1	136.81 ± 0.81
		N1 –O1 –Cl2	75.12 ± 0.64
		N2 –O2 –Cl1	75.49 ± 0.64
		N1 –C1 –C2	111.55 ± 1.10
		N1 –C1 –C3	125.01 ± 1.16
		C3 –C1 –C2	123 33 ± 1.15
		C4 –C2 –C1	121.24 ± 1.15
		N2 –O2 –Cl2	164.74 ± 0.78
		C1 –C2 –N2	113.88 ± 1.14
		N2 –C2 –C4	124.79 ± 1.21
		O2 –N2 –C2	117.11 ± 1.08
		O1 –N1 –C1	113.50 ± 1.05

a subsequent refinement was performed with the combined sets of data. The final R-value was 0.149. An absorption correction was performed but due to the small size of the crystals and the low value of the linear absorption coefficient no better results were obtained.

The fractional atomic parameters and standard deviations are given in Table 2, relevant bond distances and angles in Tables 3 and 4 and the observed and calculated structure factors in Table 5.

Table 4. Intramolecular plane angles and plane-atom distances in $Cu(H_2D)Cl_2$.

Atoms defining the plane	Plane No.	Least squares plane
Cu – Cl1 – Cl2	1	$-0.093554x+0.789509y-0.606567z=-4.593323$
Cu – N1 – N2	2	$-0.142987x+0.888244y-0.436552z=-4.048918$
Cl1 – Cl2 – N1 – N2	3	$-0.124397x+0.843199y-0.523011z=-4.502728$
O1 – C3 – C4 – O2	4	$-0.179343x+0.853762y-0.488801z=-4.419835$

Angles between the planes

plane 1 – plane 2	11.6351°
plane 1 – plane 3	5.9610°
plane 1 – plane 4	9.1332°
plane 2 – plane 3	5.6885°
plane 2 – plane 4	4.1484°
plane 3 – plane 4	3.7581°

Plane-atom distances

plane 1 – Cu	0.000014 Å
– Cl1	0.000018
– Cl2	0.000002
plane 2 – Cu	–0.000046
– N1	0.000033
– N2	0.000006
plane 3 – Cl1	–0.011432
– Cl2	0.011889
– N1	–0.016277
– N2	0.015817
– Cu	0.151783
plane 4 – O1	–0.035735
– C3	0.060111
– C4	–0.059448
– O2	0.035067
– Cu	0.083386
– N1	–0.055349
– N2	0.079381

All calculations, including the Lorentz and polarization correction, were performed on the IBM 360/50 computer at the Göteborg Computing Center for Research and Education, using programmes originally written by Coppens *et al.*[12]

DESCRIPTION OF THE STRUCTURE AND DISCUSSION

The structure is built up from double chains of copper dimethylglyoxime dichloride dimers. The two molecules of the dimer are related by an inversion center at $(0,0,\frac{1}{2})$. The molecular plane is normal to the yz-plane and the chains of dimers, held together by hydrogen bonds, extend parallel to the x-axis.

The copper atom is coordinated by an almost coplanar arrangement of two nitrogen atoms and two chlorine atoms within the molecule and to one chlorine atom, at the apex of a square pyramid, belonging primarily to the

Table 5. Observed and calculated structure factors for copper dimethylglyoxime dichloride.

h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}
0	0	1	31	-25	-1	-8	-1	88	77	-1	-5	0	438	405	-2	2	-4	77	-80	-2	-2	8	79	-114
0	0	2	38	3	-1	-7	-1	140	121	-1	-4	0	804	755	-2	0	-4	588	419	-3	8	-2	56	-70
0	0	3	136	126	-1	-6	-1	92	77	-1	-3	0	462	482	-2	1	-4	570	406	-3	4	-2	169	-175
0	0	4	256	236	-1	-5	-1	162	-161	-1	-2	0	261	328	-2	-1	-4	140	355	-3	3	-2	609	-603
0	0	5	179	-168	-1	-4	-1	74	-93	-1	-9	1	123	-116	-2	-2	-4	53	80	-3	2	-2	496	-462
0	0	7	55	44	-1	-3	-1	246	-199	-1	-7	1	65	56	-2	-3	-4	190	158	-3	1	-2	322	-315
0	1	0	568	864	-1	-2	-1	102	-116	-1	-6	1	78	-88	-2	-4	-4	156	110	-3	0	-2	187	-179
0	2	-1	604	-424	-1	1	-1	325	-296	-1	-5	1	96	-80	-2	-5	-4	112	50	-3	-1	-2	233	-213
0	3	-2	857	-737	-1	2	-1	225	161	-1	-4	1	163	-145	-2	7	-5	121	-184	-3	-2	-2	482	-403
0	4	-3	486	502	-1	3	-1	44	-49	-1	-3	1	182	-190	-2	6	-5	233	-264	-3	-3	-2	330	-282
0	5	-4	361	371	-1	4	-1	193	-144	-1	-2	1	176	-172	-2	5	-5	267	-284	-3	-4	-2	138	-191
0	6	-5	252	-349	-1	5	-1	281	-256	-1	-1	1	79	-93	-2	4	-5	124	-96	-3	-5	-2	279	-294
0	7	-6	85	-131	-1	6	-1	113	-95	-1	0	1	442	-387	-2	1	-5	484	-322	-3	-6	-2	303	-279
0	8	-7	131	184	-1	-8	-2	129	-104	-1	-7	2	219	-252	-2	0	-5	502	-354	-3	-2	-1	30	-39
0	1	1	414	-311	-1	-7	-2	269	-195	-1	-6	2	310	-363	-2	-1	-5	327	-263	-3	-3	-1	38	-53
0	2	0	43	27	-1	-6	-2	142	-114	-1	-5	2	182	-204	-2	-2	-5	192	-174	-3	-4	-1	64	-47
0	3	-1	154	171	-1	-3	-2	382	-373	-1	-4	2	207	-244	-2	-3	-5	204	-149	-3	-5	-1	72	92
0	3	0	51	-7	-1	-2	-2	1282	-926	-1	-3	2	688	-586	-2	-4	-5	302	-211	-3	-1	-1	55	-79
0	4	-1	72	-69	-1	-1	-2	721	-623	-1	-2	2	496	-420	-2	-5	-5	157	-106	-3	8	-3	91	99
0	5	-2	68	61	-1	0	-2	238	-253	-1	0	2	384	268	-2	6	-6	103	93	-3	7	-3	80	65
0	6	-3	50	42	-1	1	-2	518	-478	-1	1	2	78	-82	-2	5	-6	152	186	-3	4	-3	184	218
0	7	-4	76	-87	-1	2	-2	466	-456	-1	-8	3	113	172	-2	3	-6	145	-169	-3	3	-3	467	396
0	9	-6	55	62	-1	3	-2	144	-176	-1	-7	3	131	137	-2	2	-6	156	-147	-3	2	-3	538	531
0	1	3	112	124	-1	5	-2	79	76	-1	-6	3	155	182	-2	1	-6	91	-84	-3	1	-3	161	149
0	2	2	426	-346	-1	6	-2	143	-179	-1	-5	3	228	228	-2	-1	-6	102	-84	-3	0	-3	313	263
0	3	1	94	75	-1	7	-2	329	-274	-1	-4	3	261	296	-2	8	-7	83	143	-3	-1	-3	345	290
0	4	0	252	243	-1	8	-2	220	-231	-1	-3	3	315	316	-2	7	-7	94	116	-3	-2	-3	300	213
0	5	-1	217	-194	-1	-7	-3	64	38	-1	-2	3	373	340	-2	4	-7	94	73	-3	-4	-3	106	-106
0	6	-2	65	-55	-1	-4	-3	80	-60	-1	1	3	121	141	-2	3	-7	329	247	-3	-5	-3	69	-62
0	7	-3	156	160	-1	-3	-3	240	238	-1	-9	4	89	102	-2	2	-7	276	213	-3	-6	-3	194	145
0	9	-5	75	-68	-1	-2	-3	310	315	-1	-5	4	255	262	-2	1	-7	205	176	-3	6	-4	108	108
0	1	4	69	82	-1	-1	-3	591	493	-1	-4	4	119	109	-2	0	-7	181	139	-3	5	-4	295	301
0	2	3	132	124	-1	0	-3	410	405	-1	-3	4	134	-135	-2	-1	-7	232	158	-3	4	-4	145	134
0	3	2	219	-231	-1	1	-3	159	169	-1	-2	4	271	-231	-2	-2	-7	262	189	-3	3	-4	98	96
0	5	0	243	225	-1	2	-3	178	186	-1	-1	4	80	89	-2	-3	-7	120	77	-3	1	-4	139	131
0	6	-1	150	-155	-1	3	-3	356	390	-1	0	4	406	343	-2	-1	-8	100	-103	-3	0	-4	251	209
0	7	-2	163	-100	-1	4	-3	58	80	-1	1	4	457	416	-2	8	-8	62	-94	-3	-1	-4	136	117
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0	3	3	74	85	-1	-6	-4	112	89	-1	-6	5	169	-236	-2	0	-9	109	-103	-3	-5	-4	157	113
0	4	2	137	-135	-1	-5	-4	275	202	-1	-5	5	240	-254	-2	-3	0	387	352	-3	6	-5	164	-199
0	6	0	153	143	-1	-4	-4	205	154	-1	-4	5	183	-186	-2	-4	0	569	472	-3	5	-5	271	-314
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0	8	-1	109	-88	-1	4	-4	133	150	-1	-2	6	115	-121	-2	0	0	462	571	-3	-4	-5	358	-229
0	1	7	148	134	-1	7	-4	88	-104	-1	-1	6	206	-168	-2	-1	0	128	97	-3	-5	-5	212	-179
0	2	6	154	-143	-1	9	-4	63	89	-1	-8	7	91	126	-2	-2	0	424	-237	-3	7	-6	55	-87
0	3	5	94	-172	-1	-5	-5	108	-82	-1	-7	7	109	115	-2	4	1	88	-68	-3	4	-6	46	55
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0	6	2	222	-197	-1	-3	-5	81	-58	-1	-3	7	206	194	-2	2	1	87	93	-3	0	-6	75	-72
0	7	1	87	74	-1	-1	-5	219	-194	-1	-2	7	315	271	-2	1	1	64	47	-3	-1	-6	312	-279
0	8	0	121	109	-1	0	-5	371	-351	-1	-7	8	92	-120	-2	0	1	432	-252	-3	-2	-6	279	-191
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0	3	6	105	-85	-1	3	-5	138	-184	-2	4	-1	201	-205	-2	-5	1	324	-389	-3	7	-7	98	158
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0	5	4	228	162	-1	5	-5	194	-260	-2	2	-1	86	-89	-2	5	2	82	72	-3	5	-7	76	79
0	6	3	109	121	-1	6	-5	88	-112	-2	1	-1	416	-319	-2	3	2	433	-389	-3	4	-7	199	205
0	7	2	257	-170	-1	9	-5	108	-120	-2	0	-1	93	-151	-2	2	2	481	-395	-3	3	-7	199	201
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0	1	-9	96	-113	-1	-2	-6	141	-111	-2	-2	-1	456	408	-2	0	2	553	-427	-3	1	-7	48	38
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0	5	5	170	-175	-1	1	-6	87	91	-2	-4	-1	132	-126	-2	-2	2	443	-381	-3	-1	-7	199	148
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0	2	-2	1349	-1589	-1	-2	-7	105	97	-2	5	-2	142	-140	-2	3	3	92	80	-3	5	-8	56	-68
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0	2	-3	401	329	-1	2	-7	238	216	-2	2	-2	390	-341	-2	0	3	100	81	-3	1	-8	150	140
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0	5	-5	319	-345	-1	3	-8	156	-148	-2	-4	-2	177	-197	-2	-6	3	172	260	-3	1	-9	126	-115
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0	1	-5	186	-200	-1	6	-9	88	-141	-2	6	-3	138	182	-2	-1	5	350	-317	-3	7	-1	45	-41
0	6	-6	123	-157	-1	6	0	414	359	-2	5	-3	202	251	-2	-2	5	144	-153	-3	6	-1	129	-97
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0	2	-6	56	-51	-1	2	0	282	-159	-2	2	-3	239	166	-2	-5	5	142	-293	-3	3	-1	127	98
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0	1	-7	54	38	-1	2	2	749	-511	-2	5	-4	206	257	-2	7	2	71	-96	-3	1	0	744	731
0	7	-8	64	-90	-1	4	5	111	-88	-2	4	-4	63	54	-2	5	4	127	106	-3	0	0	641	715
0	3	-8	108	-107	-1	-9	0	147	115	-2	3	-4	221	-186	-2	4	5	60	-45	-3	-1	0	427	448

Table 5. Continued.

h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}	n	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}
-3	-2	0	302	244	-4	6	-5	125	-121	-4	2	3	47	53	-5	2	-8	78	69	-6	-3	-4	272	293
-3	-3	0	173	149	-4	5	-5	135	-135	-4	1	3	35	-19	-5	0	-8	182	-142	-6	-4	-4	244	213
-3	-4	0	434	339	-4	4	-5	95	-104	-4	0	3	28	-24	-5	-1	-8	146	-114	-6	-5	-4	117	97
-3	3	1	49	36	-4	3	-5	31	-34	-4	-1	3	118	116	-5	5	-9	54	-81	-6	6	-5	89	-123
-3	2	1	110	-70	-4	2	-5	184	-193	-4	-2	3	303	264	-5	4	-9	64	-78	-6	5	-5	174	-169
-3	1	1	379	-257	-4	1	-5	488	-474	-4	-3	3	204	203	-5	3	-9	52	-48	-6	4	-5	43	-24
-3	0	1	242	-197	-4	0	-5	494	-489	-4	-4	3	127	142	-5	2	-9	52	-47	-6	3	-5	105	-88
-3	-1	1	159	-130	-4	-1	-5	80	-66	-4	-5	3	189	219	-5	1	-9	156	-130	-6	2	-5	200	-227
-3	-2	1	360	-288	-4	-2	-5	50	-49	-4	-6	3	205	239	-5	0	-9	125	-80	-6	1	-5	222	-249
-3	-4	1	154	-131	-4	-3	-5	144	-132	-4	-7	3	82	95	-5	2	-10	98	128	-6	0	-5	126	-120
-3	-5	1	121	-136	-4	-4	-5	191	-127	-4	3	4	37	18	-5	1	-10	78	98	-6	-3	-5	234	-181
-3	6	2	95	-83	-4	-5	-5	113	-82	-4	2	4	179	107	-5	5	-1	51	-56	-6	-4	-5	255	-196
-3	5	2	129	-88	-4	4	-6	161	-185	-4	1	4	217	166	-5	2	-1	281	-231	-6	-5	-5	119	-114
-3	4	2	167	-115	-4	3	-6	102	-106	-4	0	4	268	188	-5	1	-1	322	-298	-6	4	-6	60	58
-3	3	2	223	-165	-4	2	-6	101	101	-4	-2	4	87	-40	-5	0	-1	145	-129	-6	3	-6	61	47
-3	2	2	62	-75	-4	1	-6	127	125	-4	-4	4	84	84	-5	-1	-1	104	88	-6	2	-6	88	85
-3	0	2	36	-48	-4	0	-6	69	66	-4	-5	4	96	95	-5	-2	-1	257	308	-6	0	-6	150	-132
-3	-1	2	549	-491	-4	-2	-6	219	-156	-4	-6	4	39	53	-5	-3	-1	49	31	-6	-1	-6	269	-213
-3	-2	2	631	-600	-4	-3	-6	116	-90	-4	2	5	44	-38	-5	-4	-1	83	-78	-6	-2	-6	132	-118
-3	-3	2	405	-360	-4	-4	-6	110	-74	-4	1	5	185	-133	-5	6	0	33	58	-6	-5	-6	47	-22
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-3	-6	3	99	124	-4	-1	-7	233	155	-4	-1	6	76	-64	-5	-4	0	337	342	-6	5	-8	51	-79
-3	-7	3	115	146	-4	-2	-7	209	141	-4	-2	6	109	-104	-5	-5	0	240	288	-6	4	-8	90	-111
-3	4	4	133	91	-4	-3	-7	101	80	-4	-4	6	78	74	-5	5	1	42	-41	-6	3	-8	50	-51
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-3	1	4	126	92	-4	3	-8	142	-133	-4	-3	7	37	43	-5	1	1	86	-90	-6	-1	-8	66	-65
-3	-2	4	71	-64	-4	2	-8	110	-91	-4	-6	7	45	68	-5	0	1	105	75	-6	-2	-8	50	-48
-3	-3	4	150	158	-4	1	-8	51	-45	-5	7	-2	36	-46	-5	-1	1	190	168	-6	2	-9	80	-91
-3	-4	4	291	305	-4	0	-8	55	34	-5	6	-2	97	-81	-5	-2	1	39	44	-6	1	-9	125	-134
-3	-5	4	164	187	-4	-2	-8	36	27	-5	5	-2	148	-105	-5	-3	1	141	-124	-6	0	-9	96	-95
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-3	2	5	42	-32	-4	6	-9	75	-93	-5	3	-2	183	-170	-5	-5	1	164	-195	-6	5	-2	55	-53
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-3	0	5	153	-109	-4	4	-9	62	-70	-5	1	-2	35	46	-5	3	2	141	-109	-6	3	-2	231	-190
-3	-1	5	106	-92	-4	2	-9	79	-58	-5	0	-2	181	-227	-5	2	2	223	-148	-6	2	-2	228	-209
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-3	-6	5	63	-62	-4	5	-10	46	77	-5	7	-3	44	50	-5	-3	2	41	-44	-6	4	-1	95	72
-3	1	6	51	-34	-4	4	-10	56	61	-5	5	-3	122	96	-5	-5	2	96	-111	-6	3	-1	124	97
-3	-4	6	83	101	-4	3	-10	54	47	-5	4	-3	267	283	-5	-6	2	116	-155	-6	1	-1	229	-200
-3	-6	6	64	-95	-4	2	-10	31	26	-5	3	-3	244	279	-5	-7	2	119	-167	-6	0	-1	45	-24
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-3	-1	7	53	55	-4	6	-1	160	-136	-5	1	-3	34	-10	-5	2	3	134	80	-6	-2	-1	113	-107
-3	-2	7	58	66	-4	5	-1	178	-142	-5	0	-3	104	-85	-5	1	3	63	39	-6	-3	-1	165	-137
-3	-3	7	60	68	-4	4	-1	128	-113	-5	-1	-3	173	194	-5	0	3	138	98	-6	-4	-1	54	-41
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-4	7	-2	113	-118	-4	0	-1	29	-43	-5	-5	-3	120	129	-5	-4	3	35	15	-6	2	0	179	138
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-4	2	-2	241	-238	-4	5	0	286	212	-5	5	-4	67	47	-5	1	4	77	70	-6	-2	0	28	-24
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-4	0	-2	312	-473	-4	2	0	139	144	-5	2	-4	174	173	-5	-1	4	100	73	-6	-4	0	169	183
-4	-1	-2	277	-434	-4	1	0	270	231	-5	1	-4	321	291	-5	-2	4	46	23	-6	-5	0	121	125
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-4	-3	-2	129	-147	-4	-1	0	319	325	-5	-1	-4	252	207	-5	-4	4	132	137	-6	3	1	45	49
-4	-4	-2	123	-120	-4	-2	0	348	388	-5	-2	-4	272	227	-5	-6	4	47	-51	-6	2	1	120	-99
-4	-3	-1	235	-210	-4	-3	0	347	331	-5	-3	-4	133	130	-5	0	5	98	-100	-6	1	1	209	-180
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-4	7	-3	114	110	-4	5	1	69	-57	-5	5	-5	163	-164	-5	-3	5	91	-96	-6	-3	1	78	-81
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-4	3	-3	184	189	-4	1	1	108	-110	-5	0	-5	261	-249	-6	3	-3	260	234	-6	-1	2	209	-170
-4	2	-3	113	127	-4	0	1	294	-210	-5	-1	-5	123	-126	-6	2	-3	48	38	-6	-2	2	252	-215
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-4	-1	-3	424	456	-4	-2	1	115	-87	-5	-4	-5	319	-235	-6	0	-3	171	219	-6	-4	2	39	41
-4	-2	-3	556	597	-4	-3	1	332	-298	-5	-5	-5	87	-46	-6	-1	-3	169	258	-6	-6	2	93	-106
-4	-3	-3	108	98	-4	-4	1	355	-303	-5	6	-6	78	98	-6	-2	-3	117	119	-6	-7	2	53	-72
-4	-4	-3	81	-56	-4	-6	1	144	192	-5	5	-6	93	108	-6	-3	-3	60	-41	-6	0	3	115	93
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-4	5	-4	48	57	-4	4	2	262	-164	-5	3	-6	110	-119	-6	-5	-3	69	62	-6	-2	3	180	163
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-4	-1	-4	27	-7	-4	-2	2	272	-246	-5	-3	-6	80	64	-6	6	-4	80	89	-6	-4	4	100	116
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-4	-3	-4	57	27	-4	-4	2	232	-194	-5	4	-7	107	104	-6	4	-4	125	100	-6	-6	4	35	-43
-4	-4	-4	299	252	-4	-5	2	39	-129	-5	3	-7	216	191	-6	3	-4	73	66	-6	-3	5	99	-135
-4	-5	-4	277	187	-4	-6	2	42	-170	-5	2	-7	215	172	-6	2	-4	52	-41	-6	-4	5	90	-132
-4	-6	-4	133	111	-4	-7	2	121	-136	-5	1	-7	118	98	-6	0	-4	25	34	-6	-5	5	39	-53
-4	8	-5	38	-50	-4	4	3	49	40	-5	0	-7	76	61	-6	-1	-4	39	51	-1	0	0	588	627
-4	7	-5	50	-46	-4	3	3	176	126	-5	-1	-7	333	219	-6	-2	-4	188	183	-2	0	0	509	521
										-5	-2	-7	274	182										

Table 5. Continued.

h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}
-3	0	0	777	715	5	1	-2	126	-177	-1	1	3	122	141	-2	2	-7	189	213	-3	3	-4	90	96
-4	0	0	277	338	4	1	-2	105	-129	-2	1	3	321	268	-3	2	-7	115	115	-4	3	-4	144	135
-5	0	0	197	252	3	1	-2	454	-491	8	1	4	71	69	-4	2	-7	221	251	-5	3	-4	99	-107
-6	0	0	234	263	2	1	-2	597	-621	6	1	4	75	51	-5	2	-7	184	172	-7	3	-4	164	127
-7	0	0	119	120	0	1	-2	460	-496	5	1	4	231	207	2	2	-8	125	-114	6	3	-5	135	-135
-6	0	1	110	-104	-1	1	-2	517	-478	3	1	4	114	117	-1	2	-8	120	-117	5	3	-5	93	-96
-5	0	1	80	75	-2	1	-2	121	91	2	1	4	409	355	-4	2	-8	82	-91	3	3	-5	157	-191
-4	0	1	200	-210	-3	1	-2	355	-315	1	1	4	130	128	-5	2	-10	99	129	0	3	-5	207	-229
-3	0	1	154	-197	-4	1	-2	329	-275	-1	1	4	557	416	7	2	0	174	164	-1	3	-5	147	-184
-2	0	1	250	-252	-6	1	-2	159	-157	-2	1	4	271	245	5	2	0	138	153	-3	3	-5	133	-147
-1	0	1	388	-387	-7	1	-2	218	-169	5	1	5	95	-126	4	2	0	493	388	-6	3	-5	101	-88
1	0	1	63	-71	6	1	-3	203	192	4	1	5	64	-66	3	2	0	318	244	-1	3	-6	163	-179
2	0	1	115	-151	5	1	-3	114	133	2	1	5	249	-263	2	2	0	522	-237	-2	3	-6	154	-169
3	0	1	727	-566	4	1	-3	82	116	1	1	5	189	-194	1	2	0	300	328	-4	3	-6	95	-106
5	0	1	127	-129	3	1	-3	260	288	0	1	5	108	-93	6	2	1	115	-107	-5	3	-6	107	-119
-6	0	2	87	-64	2	1	-3	60	85	-1	1	5	160	-150	5	2	1	400	348	2	3	-7	244	231
-5	0	2	144	-107	1	1	-3	331	306	8	1	6	68	-85	4	2	1	256	198	1	3	-7	176	194
-2	0	2	385	-427	-1	1	-3	155	169	6	1	6	230	-213	2	2	1	616	408	0	3	-7	129	133
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0	0	2	85	3	-4	1	-3	83	-87	2	1	6	72	-84	7	2	2	143	-146	-2	3	-7	247	247
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2	0	3	236	-178	4	1	-5	73	-36	2	1	8	91	-103	4	2	3	716	597	5	3	0	319	299
3	0	3	282	263	3	1	-5	95	-92	7	2	-1	99	-78	3	2	3	265	213	4	3	0	385	371
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7	0	3	126	110	0	1	-5	167	-200	1	2	-1	113	-172	0	2	3	185	124	1	3	0	362	482
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7	0	7	91	70	5	1	1	98	88	-5	2	-4	152	173	1	3	-2	505	-586	3	3	5	74	-82
8	0	7	130	132	4	1	1	296	253	-7	2	-4	204	183	0	3	-2	684	-737	2	3	5	175	-149
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-2	1	0	848	848	1	1	3	691	493	0	2	-7	110	95	-1	3	-4	140	119	2	4	-3	45	71
6	1	-2	151	-170	0	1	3	121	124	-1	2	-7	186	216	-2	3	-4	215	-186	1	4	-3	251	296

Table 5. Continued.

h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}	h	k	l	F_{obs}	F_{calc}
0	4	-3	415	502	8	4	4	83	62	9	5	3	59	66
-1	4	-3	62	86	7	4	4	147	119	8	5	3	85	83
-2	4	-3	267	321	6	4	4	276	213	6	5	3	84	62
-3	4	-3	201	218	4	4	4	313	252	5	5	3	153	129
-4	4	-3	102	120	3	4	4	385	298	3	5	3	83	-62
-5	4	-3	349	283	2	4	4	164	110	2	5	3	57	59
6	4	-4	99	116	1	4	4	237	154	1	5	3	64	-44
5	4	-4	121	137	0	4	4	380	215	7	5	4	92	85
4	4	-4	80	94	9	4	5	78	-80	6	5	4	133	97
3	4	-4	275	305	8	4	5	65	-73	4	5	4	269	197
2	4	-4	105	127	7	4	5	151	-104	3	5	4	187	113
1	4	-4	95	109	6	4	5	270	-196	2	5	4	147	52
0	4	-4	589	633	5	4	5	357	-235	1	5	4	341	202
-1	4	-4	147	150	4	4	5	195	-127	0	5	4	267	162
-3	4	-4	144	134	3	4	5	364	-229	6	5	5	104	-114
-4	4	-4	61	59	2	4	5	334	-211	5	5	5	91	-46
-6	4	-4	156	100	1	4	5	111	-74	4	5	5	130	-87
6	4	-5	123	-132	0	4	5	295	-184	3	5	5	259	-179
5	4	-5	64	-65	7	4	6	67	-58	2	5	5	191	-106
4	4	-5	169	-178	4	4	6	94	-74	1	5	5	157	-82
3	4	-5	222	-236	3	4	6	106	70	7	5	6	75	-67
2	4	-5	194	-237	7	4	7	66	61	5	5	6	62	-50
1	4	-5	172	-186	3	4	7	66	49	4	5	6	82	-79
0	4	-5	271	-288	7	5	-2	82	-84	2	6	-4	89	-113
-1	4	-5	113	-127	5	5	-2	104	-111	2	6	-3	237	260
-2	4	-5	117	-96	4	5	-2	109	-129	2	6	-2	188	-198
-3	4	-5	294	-315	1	5	-2	118	-204	3	6	-3	125	124
-4	4	-5	84	-104	0	5	-2	48	61	3	6	-2	144	-132
-5	4	-5	95	-86	-1	5	-2	71	76	4	6	-5	108	-112
4	4	-6	70	74	-2	5	-2	150	-140	4	6	-3	230	239
3	4	-6	86	101	7	5	-3	142	146	4	6	-2	172	-170
1	4	-6	133	159	4	5	-3	173	219	5	6	-3	268	271
0	4	-6	80	88	2	5	-3	102	121	5	6	-2	155	-155
-4	4	-6	167	-185	1	5	-3	190	228	6	6	-2	113	-106
-6	4	-6	83	58	-2	5	-3	219	251	7	6	-2	95	-99
-7	4	-6	119	-101	-5	5	-3	148	96	7	6	-3	92	109
2	4	-7	107	122	6	5	-4	82	101	1	6	-5	204	-236
0	4	-7	124	123	4	5	-4	100	95	1	6	-4	72	98
-1	4	-7	300	282	3	5	-4	197	197	1	6	-3	150	182
-2	4	-7	77	73	2	5	-4	68	75	0	6	-7	113	133
-3	4	-7	216	205	1	5	-4	273	262	0	6	-6	107	-157
-4	4	-7	205	173	0	5	-4	317	371	0	6	-5	288	-349
-5	4	-7	111	104	-2	5	-4	210	257	0	6	-2	49	-55
-6	4	-7	152	146	-3	5	-4	308	301	0	6	-1	167	-155
-7	4	-7	156	140	-6	5	-4	118	93	-1	6	-9	106	-141
-3	4	-8	107	-104	4	5	-5	167	-170	-1	6	-5	115	-112
-4	4	-8	130	-149	3	5	-5	256	-257	-1	6	-3	151	134
-6	4	-8	88	-111	2	5	-5	185	-203	-1	6	-2	157	-179
-7	4	-8	66	-75	1	5	-5	253	-254	-1	6	-1	114	-95
1	4	-9	108	-121	0	5	-5	305	-345	-2	6	-6	104	93
-1	4	-9	66	-73	-1	5	-5	279	-260	-2	6	-5	229	-264
-2	4	-9	75	-76	-2	5	-5	297	-284	-2	6	-4	190	197
-4	4	-9	67	-79	-3	5	-5	258	-314	-2	6	-3	135	182
-5	4	-9	67	-78	-4	5	-5	131	-135	-2	6	-2	147	-119
-4	4	-10	49	61	-5	5	-5	176	-164	-3	6	-7	109	121
-2	4	-1	199	-205	-6	5	-5	217	-169	-3	6	-5	191	-199
-1	4	-1	170	-144	1	5	-6	154	175	-3	6	-4	112	108
8	4	-1	96	-103	0	5	-6	81	86	-4	6	-5	155	-121
7	4	-1	122	-108	-2	5	-6	167	186	-4	6	-3	136	95
5	4	-1	436	-373	-5	5	-6	108	108	-5	6	-6	106	98
4	4	-1	371	-303	3	5	-7	81	78	-5	6	-5	231	-211
3	4	-1	136	-131	0	5	-7	110	91	-5	6	-4	99	64
2	4	-1	302	-390	-3	5	-7	93	79	-6	6	-5	142	-123
1	4	-1	69	-145	1	5	-9	75	-103	4	6	-1	182	192
0	4	-1	50	-69	-1	5	-9	116	-149	3	6	-1	67	-93
8	4	0	203	166	-2	5	-9	101	-116	2	6	-1	53	-81
7	4	0	177	158	-4	5	-9	118	-138	1	6	-1	50	-88
6	4	0	189	183	-5	5	-9	65	-81	6	6	0	87	86
5	4	0	368	342	-2	5	-1	107	-89	5	6	0	149	166
4	4	0	354	300	-1	5	-1	308	-256	4	6	0	116	121
3	4	0	356	339	5	5	-1	185	-195	3	6	0	141	135
2	4	0	378	472	3	5	-1	120	-136	2	6	0	210	213
1	4	0	320	755	2	5	-1	277	-389	0	6	0	236	143
0	4	0	293	243	1	5	-1	58	-80	6	6	1	221	172
-1	4	0	459	421	0	5	-1	206	-194	5	6	1	148	109
7	4	1	147	-129	8	5	0	83	92	4	6	1	190	132
6	4	1	49	-41	7	5	0	93	94	3	6	1	205	174
5	4	1	80	-78	6	5	0	157	125	1	6	1	86	77
4	4	1	509	-437	5	5	0	321	288	0	6	1	107	74
3	4	1	70	-47	4	5	0	222	197	8	6	2	113	-87
2	4	1	133	-126	3	5	0	323	275	7	6	2	172	-132
1	4	1	97	-93	2	5	0	477	501	6	6	2	234	-210
-1	4	1	148	-131	1	5	0	429	405	5	6	2	73	-46
9	4	2	59	-62	0	5	0	307	225	4	6	2	307	-222
8	4	2	123	-107	-1	5	0	622	505	3	6	2	373	-279
6	4	2	180	-164	9	5	1	58	77	2	6	2	185	-130
5	4	2	214	-235	6	5	1	100	87	1	6	2	154	-114
4	4	2	134	-120	4	5	1	93	-77	7	6	3	79	57
3	4	2	178	-191	3	5	1	83	92	6	6	3	202	142
2	4	2	216	-197	2	5	1	134	-109	5	6	3	279	189
0	4	2	183	-135	1	5	1	233	-161	4	6	3	79	32
-1	4	2	524	-379	-1	5	1	89	-37	3	6	3	251	145
8	4	3	59	54	9	5	2	90	-106	2	6	3	234	136
6	4	3	149	-102	8	5	2	124	-111	7	6	4	72	75
5	4	3	91	-61	7	5	2	86	-72	4	6	4	142	111
4	4	3	72	-56	6	5	2	327	-257					
3	4	3	125	-106	5	5	2	147	-138					
2	4	3	117	131	3	5	2	338	-294					
-1	4	3	108	45	2	5	2	192	-159					
9	4	4	130	113	0	5	2	171	-125					

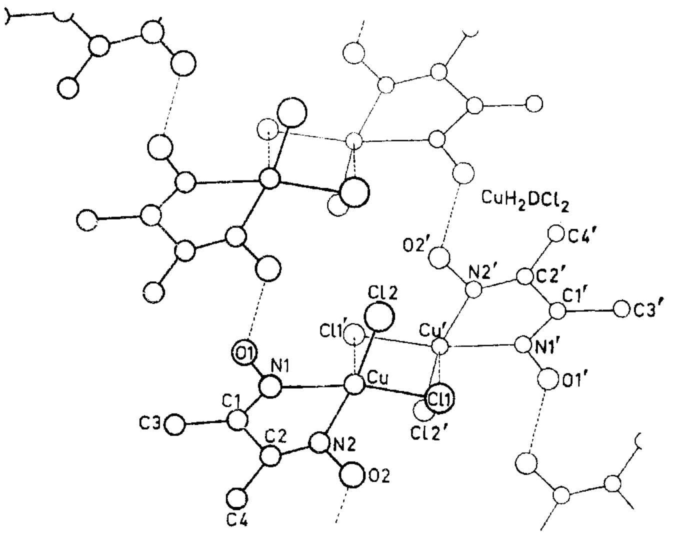

Fig. 2. A projection of the structure of copper dimethylglyoxime dichloride. The two molecules of the dimer are related by an inversion center at (0,0,½), *i.e.* midway between the copper atoms Cu and Cu′.

adjacent molecule. The dimer thus formed is in this way held together by two copper-chlorine-copper bridges as is shown in Fig. 2 (Cu—Cl1′—Cu′ and Cu′—Cl1—Cu). The copper atom is displaced 0.15 Å out of the molecular plane in the direction of chlorine atom (Cl1′) of the neighbouring molecule. The mean copper-nitrogen distance is 1.99 Å and the mean intramolecular copper-chlorine distance is 2.24 Å. The third chlorine atom is coordinated by a weak bond of length 2.70 Å.

The presence of an intra-molecular hydrogen bond was indicated by the IR spectrum. The chlorine atom labelled Cl2 is only bound to one copper atom and should therefore have the most pronounced electron donor properties. The distance between O1 and Cl2 (3.03 Å) is shorter than that between O2 and Cl1 (3.12 Å). This might suggest the presence of a hydrogen bond between O1 and Cl2. The inter-molecular distance (2.90 Å) between the oxygen atoms O1 and O2 indicates the position of the other hydrogen bond seen in the IR-spectrum.

The hydrogen atoms appear to be in fixed positions, otherwise the IR peaks would not be sharp. The N1—O1—Cl2 and N2—O2—O1 angles are 75° and 136°, respectively. The N—O—H angles should be approximately 108°, which means that the hydrogen bonds cannot be linear.

Relevant bond distances and angles are shown in Fig. 3 a, b.

Copper dichloride compounds have often been found to polymerise as a result of the electron donor properties of the chlorine atoms, to form chains of the type found in $CuCl_2$. The copper atom is thus four-coordinated, by a coplanar arrangement of ligands and two possible further ligands can be,

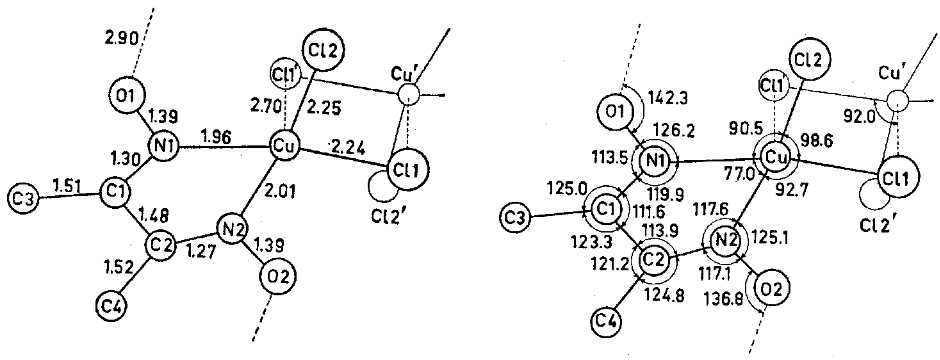

Fig. 3a. Bond distances in Å for copper dimethylglyoxime dichloride. *3b.* Bond angles.

so as to say, attached perpendicular to the plane by weak bonds to form a distorted octahedral configuration about the copper atom. As long as the two chlorine atoms are ligands in *trans*-positions within the complex, they can both participate in bridging. This has been reported for dimethylnitrosamine-copper(II) dichloride [13] and dipyridine-copper(II) dichloride.[14] Duckworth *et al.*[15] found, however, that the polymerisation could sometimes be reduced to dimerisation as in the structure of di(4-methylpyridine)-copper(II) dichloride, and he suggested that this was a result of steric hindrance.

Five coordination by adduct formation is reported for diacetylacetonato-copper(II) [16] with quinoline. In the discrete complex the copper atom is coordinated to the four oxygen atoms of the acetylacetone radicals forming a distorted coplanar arrangement, and to the nitrogen atom of the quinoline molecule at the apex of a square pyramid. Five-coordination has also been found in copper dimethylglyoxime, $Cu(HD)_2$, both in the crystalline state [17] and in solution.[18] The crystal structure reveals dimers of coplanar $Cu(HD)_2$ molecules with two copper-oxygen linkages per dimer. In solution monomers of $Cu(HD)_2$ form adducts with quinoline and aliphatic amines. These complexes have been studied at this university by means of EPR.[19] The nickel and copper complexes of ethylmethyloxime are also being studied [20] at the Department of Analytical Chemistry.

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