

Electron-diffraction Studies of Chlorobutatriene and Chlorobutenynes. II. Molecular Structures of Gaseous *cis*- and *trans*-1-Chlorobutenynes

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The molecular structure of *cis*- and *trans*-1-chlorobuten-3-yne have been investigated by electron diffraction from the vapour. Normal coordinate calculations based upon assumed force fields supplied amplitudes of vibration which could not be determined from the electron-diffraction data, and correction terms which were used in geometrically consistent r_a -refinements. The final bond distances (r_a -values; Å) and valence angles ($^\circ$) are:

	<i>cis</i>	<i>trans</i>
C(<i>sp</i>)-H	1.068(17)	1.090(15)
C(<i>sp</i> ²)-H	1.095(17)	1.117(15)
C≡C	1.212(6)	1.220(8)
C=C	1.345(7)	1.356(7)
C-C	1.426(6)	1.436(6)
C-Cl	1.716(5)	1.717(4)
∠C=C-C	123.9(0.6)	120.7(1.0)
∠C≡C-C	178.0(2.2)	180.2(2.4)
∠C=C-Cl	123.9(0.6)	121.1(0.8)
∠C=C ₁ -H	119.2(4.4)	124.7(4.2)
∠C=C ₂ -H	122.0 (assumed)	122.0 (assumed)
∠C≡C-H	180.0 (assumed)	180.0 (assumed)

Parenthesized values are 2σ where systematic uncertainties are included.

Electron-diffraction studies of *cis*- and *trans*-1-chlorobuten-3-yne were carried out as a part of the determination of the molecular structures of gaseous C₄H₃Cl isomers.¹

EXPERIMENTAL AND CALCULATION PROCEDURES

Pure *cis*- and *trans*-1-chlorobuten-3-yne were obtained and prevented from polymerization as described for chlorobutatriene.¹ Some, but

not severe loss of sample due to polymerization during the experiment was experienced. Electron diffraction photographs were made in the Oslo Apparatus² at nozzle-to-plate distances of 48 and 28 cm, keeping the sample reservoirs at about -12 and -15°C, respectively for the two compounds. The electron wavelength was 0.06464 Å as calibrated against diffraction patterns of gaseous benzene. The scattering functions for the 35 kV electrons were those computed for chlorobutatriene. Three plates made at each of the two camera distances were used in the investigation for both compounds. The plates were handled and the data reduced in routine fashion³ to yield the experimental modified intensities and radial distribution curves shown respectively in Figs. 1 and 3, and Figs. 2 and 4 for the two compounds. The structure analysis and supporting calculations were carried out using the standard procedures and computer programs³⁻⁵ as outlined elsewhere.¹

CALCULATIONS AND REFINEMENTS

Planar models of 1-chlorobutenyne are described by thirteen geometrical parameters; see Fig. 5. In this investigation the following restrictions were introduced: ∠C≡C-H = 180°, $r_{C_1-H} = r_{C_2-H} = r_{C_3-H} + 0.027$ Å = r_{C-H} . The ten parameters to be adjusted were then: r_{C-H} , $r_{C\equiv C}$, $r_{C=C}$, r_{C-C} , r_{C-Cl} , ∠C=C-Cl, ∠C=C-C, ∠C≡C-C (*trans* to the C=C-C angle), ∠C=C₁-H, and ∠C=C₂-H.

Force constants for similar molecules were used to design a diagonal force field for *cis*- and *trans*-chlorobutenyne; see Table 1. Normal coordinate calculations were then carried out

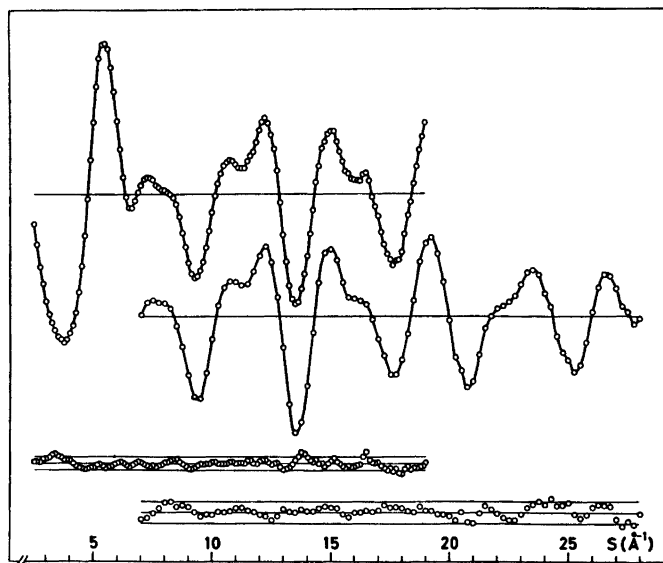


Fig. 1. Experimental intensity data for *cis*-1-chlorobutyne from the 48 cm ($\Delta s = 0.125 \text{ \AA}^{-1}$) and 28 cm ($\Delta s = 0.25 \text{ \AA}^{-1}$) camera distances. Theoretical curves are not shown, but the corresponding differences between experimental and theoretical intensities calculated according to the parameter values of Table 4, are given. The full lines given along with the differences indicate the estimated uncertainties (three standard deviations) of the experimental intensity points.

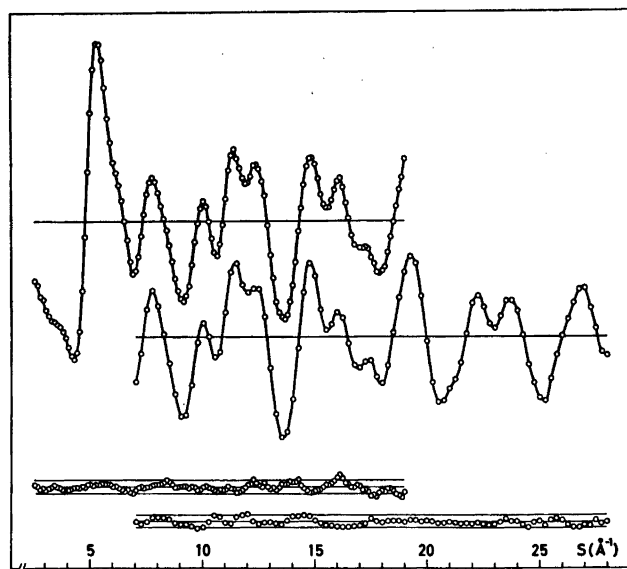


Fig. 2. Experimental intensity data for *trans*-1-chlorobutyne from the 48 cm ($\Delta s = 0.125 \text{ \AA}^{-1}$) and 28 cm ($\Delta s = 0.25 \text{ \AA}^{-1}$) camera distances. Theoretical curves are not shown, but the corresponding differences between experimental and theoretical intensities calculated according to the parameter values of Table 4, are given. The full lines given along with the differences indicate the estimated uncertainties (three standard deviations) of the experimental intensity points.

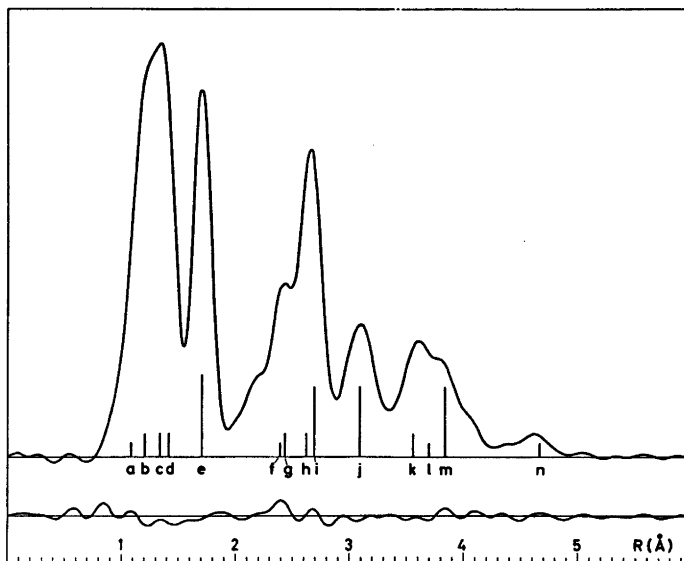


Fig. 3. Experimental radial distribution curve for *cis*-1-chlorobutyne, calculated for the artificial damping constant $k = 0.0015 \text{ \AA}^2$. The approximate positions of the important interatomic distances are indicated: a, $C(sp^2) - H$ and $C(sp) - H$; b, $C \equiv C$; c, $C = C$; d, $C - C$; e, $C - Cl$; f, $Cl \cdots H_7$; g, $C_1 \cdots C_3$; h, $C_2 \cdots C_4$; i, $C_2 \cdots Cl$; j, $C_3 \cdots Cl$; k, $C_1 \cdots C_4$; l, $Cl \cdots H_3$; m, $C_1 \cdots Cl$; n, $Cl \cdots H_5$. The difference between the experimental and theoretical radial distribution curves calculated according to the parameter values in Table 4 is also shown.

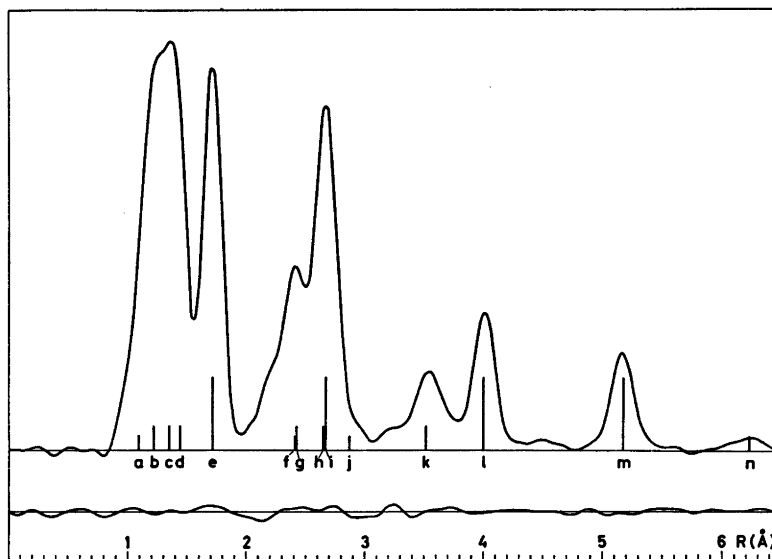


Fig. 4. Experimental radial distribution curve for *trans*-1-chlorobutyne calculated for the artificial damping constant $k = 0.0015 \text{ \AA}^2$. The approximate positions of the important interatomic distances are indicated: a, $C(sp^2) - H$ and $C(sp) - H$; b, $C \equiv C$; c, $C = C$; d, $C - C$; e, $C - Cl$; f, $Cl \cdots H_7$; g, $C_1 \cdots C_3$; h, $C_2 \cdots C_4$; i, $C_2 \cdots Cl$; j, $Cl \cdots H_3$; k, $C_1 \cdots C_4$; l, $C_3 \cdots Cl$; m, $C_4 \cdots Cl$; n, $Cl \cdots H_5$. The difference between the experimental and theoretical radial distribution curves calculated according to the parameter values in Table 4 is also shown.

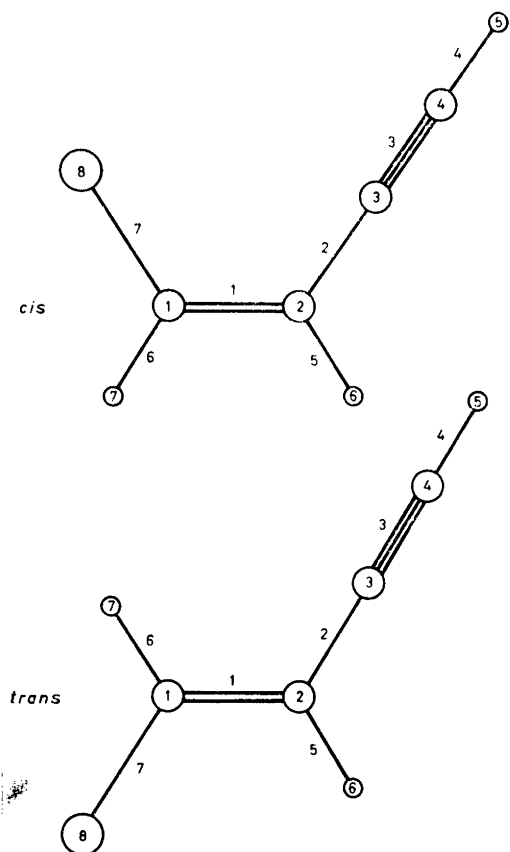


Fig. 5. Numbering of atoms and bonds in *cis*- and *trans*-1-chlorobutenyne, C_4H_3Cl .

Table 1. Force field for *cis*- and *trans*-1-chlorobuten-3-yne.^a

$K_1 = 9.1$	$K_{15} = 0.50$	$\varrho_7^{16} = 0.30$
$K_2 = 4.6$	$K_{17} = 0.85$	$\varrho_6^{17} = 0.20$
$K_3 = 15.7$	$K_{67} = 0.25$	$\varrho_6^{12} = 0.20$
$K_4 = 6.3$	$K_{15} = 0.53$	$\varrho_2^{15} = 0.25$
$K_5 = 5.4$	$K_{25} = 0.25$	$\chi_{12}^{16} = \chi_{15}^{18} = 0.12 (0.14)^c$
$K_6 = 5.6$	$K_{12} = 0.84$	$\chi_{15}^{16} = \chi_{12}^{18} = 0.14 (0.12)^c$
$K_i = 3.9$	$K_{23}^b = 0.32$	
	$K_{34}^b = 0.23$	

^a For numbering of the bonds, see Fig. 3. The meaning of the symbols: K_i , stretching of bond i ; K_{ij} , bending of angle between bonds i and j ; ϱ_k^{ij} , bending of bond k out of ij -plane; χ_{kl}^{ij} , torsion between the ij - and kl -planes. The force constants are given in $\text{mdyn}/\text{\AA}$ and $\text{mdyn}\text{\AA}/(\text{rad})^2$. ^b Identical force constants for bending in plane and out of plane are assumed. ^c Parenthesized values for *trans*.

using coordinates consistent with the models given in Table 3 where also the resulting D and l -values⁵ are given. The obtained l -values agree well with those calculated for corresponding distances in butenyne.⁶

The interpretation of the main features of the experimental radial distribution curves was straightforward as indicated by the approximate positions of the important interatomic distances (*cf.* Table 3) shown in Figs. 2 and 4, respectively, for *cis*- and *trans*-chlorobutenyne. Least-squares refinements were carried out under conditions given in Table 2. The results of r_α -refinements where the amplitudes of vibration were fixed at the calculated values and where $\angle C=C-H = 122.0^\circ$ are given in Table 3. Corresponding r_α -refinements where the D -values in Table 3 were used to obtain the geometrically consistent models⁵ did not result in significant changes in the parameter values nor in the least-squares fits. Attempts were now made to include the amplitudes of vibration in the least-squares refinements, except those corresponding to the $C\cdots H$ and $H\cdots H$ non bonded interactions. Amplitudes for overlapping distances were refined in groups. The group containing the C,C bond distances refined, however, to unreasonable values for both molecules, as was also the case for the C,H bond distances in *cis*-chlorobutenyne. These amplitudes were therefore restricted to the calculated values, which finally also was the case for the amplitudes associated with the two longest $Cl\cdots H$ distances. The results of a refinement using these restrictions on the amplitudes are given in Table 4 for *trans*-chlorobutenyne. A corresponding refinement for *cis*-chlorobutenyne revealed additional problems. The amplitudes for the two groups of amplitudes corresponding to interatomic distances at about 2.4 and 2.6 \AA both refined to unacceptable low values ($l_{C,C_1} = 0.043$, $l_{C_1,C_1} = 0.037$), and they were consequently also fixed at the calculated values. The result of this final refinement for *cis*-chlorobutenyne is given in Table 4. The least-squares fit was better for the less restricted refinement ($R = 6.37\%$), but only the values for the C-C single bond (1.417(3) \AA) and the C=C-C angle (124.7(0.3) $^\circ$) differed from those of the final model by as much as two standard deviations. Non-planar models (torsion about the C=C bond and bending

Table 2. Refinement conditions for *cis*- and *trans*-1-chlorobuten-3-yne.

	Curve (camera dist.)	Data range		Data interval	Constants of the weightscheme ^{4,5}						
		s_{\min}	s_{\max}	Δs	s_1	s_2	w_1	w_2	p_1	p_2	W
<i>cis</i> -	48 cm	2.50	19.50	0.125	6.00	15.00	0.05	0.01	-0.64	0.146	1.0
	28 cm	7.00	28.00	0.25	7.00	22.00	0.05	0.02	-0.60	0.125	0.5
<i>trans</i> -	48 cm	2.50	19.00	0.125	6.50	15.00	0.05	0.01	-0.64	0.146	1.0
	28 cm	7.00	28.00	0.25	8.00	22.00	0.05	0.02	-0.60	0.125	0.5

Table 3. Computed *D*- and *l*-values, and r_a -structure for *cis*- and *trans*-chlorobutenyne.^a

Parameters ^b	<i>cis</i>			<i>trans</i>			
	<i>D</i> -values	<i>l</i> -values	r_a -structure ^c	<i>D</i> -values	<i>l</i> -values	r_a -structure ^c	
C-H	4,5	-0.0329	0.072	1.069(8)	-0.0348	0.072	1.083(7)
	2,6	-0.0103	0.075	1.096(8)	-0.0095	0.075	1.110(7)
	1,7	-0.0117	0.074		-0.0106	0.074	1.110(7)
C≡C	3,4	-0.0104	0.036	1.210(3)	-0.0121	0.036	1.220(3)
C=C	1,2	-0.0025	0.041	1.344(3)	-0.0010	0.041	1.355(3)
C-C	2,3	-0.0024	0.048	1.423(3)	-0.0027	0.048	1.437(3)
C-Cl	1,8	-0.0027	0.047	1.716(2)	-0.0053	0.047	1.716(1)
C...C	2,4	-0.0039	0.052	2.633(4)	-0.0059	0.052	2.657(4)
	1,3	-0.0015	0.066	2.446(5)	-0.0009	0.067	2.419(5)
	1,4	-0.0002	0.086	3.574(7)	-0.0028	0.090	3.521(4)
C...Cl	2,8	-0.0005	0.067	2.699(3)	-0.0018	0.067	2.674(3)
	3,8	+0.0036	0.126	3.098(7)	-0.0005	0.069	4.013(3)
	4,8	+0.0085	0.188	3.856(14)	+0.0009	0.081	5.180(3)
Cl...H	8,7	-0.0055	0.110	2.404(27)	-0.0081	0.109	2.408(26)
	8,6	-0.0032	0.097	3.716(8)	+0.0026	0.151	2.869(6)
	8,5	+0.0053	0.259	4.637(22)	-0.0081	0.118	6.233(7)
C...H	3,5	-0.0291	0.077	2.279(9)	-0.0327	0.077	2.303(8)
	2,5	-0.0158	0.085	3.703(10)	-0.0195	0.085	3.740(8)
	1,5	-0.0081	0.127	4.605(12)	-0.0135	0.131	4.550(8)
	1,6	-0.0057	0.098	2.138(8)	-0.0033	0.098	2.159(7)
	3,6	-0.0044	0.108	2.118(8)	-0.0042	0.106	2.190(10)
	4,6	-0.0024	0.127	3.228(11)	-0.0024	0.124	3.338(10)
	2,7	-0.0076	0.098	2.127(23)	-0.0041	0.099	2.180(23)
	3,7	-0.0058	0.098	3.437(18)	+0.0011	0.147	2.716(44)
	4,7	-0.0023	0.105	4.610(15)	+0.0005	0.189	3.559(42)
	5,7	-0.0110	0.158	4.250(18)	-0.0119	0.154	4.389(16)
H...H	5,6	-0.0072	0.134	5.659(19)	-0.0088	0.241	4.456(41)
$\angle C=C-C$	-	-	124.2(0.4)	-	-	120.0(0.5)	
$\angle C\equiv C-C$	-	-	178.9(1.2)	-	-	181.9(1.1)	
$\angle C=C-Cl$	-	-	123.3(0.3)	-	-	120.7(2.2)	
$\angle C=C_1-H$	-	-	120.9(2.1)	-	-	124.1(0.3)	
$\angle C=C_2-H$	-	-	[122.0]	-	-	[122.0]	
R_w^d (%)	-	-	8.23	-	-	7.24	

^a Correction terms (*D*-values), amplitudes (*l*-values) and distances (r_a) in Ångströms; angles in degrees. The r_a -structure gives the result of r_a -refinement (no *D*-value correction) using the calculated *l*-values. ^{b,c,d} See corresponding comments under Table 4.

Table 4. Important parameter values and corresponding moments of inertia for *cis*- and *trans*-1-chlorobutenyne.^a

Parameters ^b		<i>cis</i> - r_a^c	l^c	<i>trans</i> - r_a^c	l^c
C—H	4,5	1.068(8)	[0.072]	1.090(7)	0.071(10)'
	2,6	1.095(8)	[0.075]	1.117(7)	0.074(10)'
	1,7	1.095(8)	[0.074]	1.117(7)	0.074(10)'
C≡C	3,4	1.212(3)	[0.036]	1.220(3)	[0.036]
	C=C	1,2	1.345(3)	[0.041]	[0.041]
C—C	2,3	1.426(3)	[0.048]	1.436(3)	[0.048]
C—Cl	1,8	1.716(2)	0.051(3)	1.717(1)	0.047(2)
	C···C	2,4	2.629(5)	[0.052]	2.646(5)
C···Cl	1,3	2.442(4)	[0.066]	2.424(5)	0.053(5)'''
	1,4	3.565(6)	0.082(8)	3.531(4)	0.076(7)
	2,8	2.703(3)	[0.067]	2.678(4)	0.061(3)''
	3,8	3.098(4)	0.110(5)	4.013(2)	0.064(3)
	4,8	3.857(12)	0.184(10)	5.177(3)	0.076(3)
Cl···H	8,7	2.412(28)	[0.110]	2.397(27)	0.095(5)'''
	8,6	3.710(10)	[0.097]	2.873(8)	[0.151]
	8,5	4.669(20)	[0.257]	6.215(8)	[0.118]
	$\angle C=C-C$		123.9(0.3)		120.7(0.5)
$\angle C\equiv C-C$		178.0(1.1)		180.1(1.2)	
$\angle C=C-Cl$		123.9(0.3)		121.1(0.4)	
$\angle C=C_1-H$		119.2(2.2)		124.7(2.1)	
$\angle C=C_3-H$		[122.0]		[122.0]	
R_w^d (%)		7.52		6.58	
I_a^e		(56.60) ⁸	56.2	(—) ⁷	11.1
I_b		(196.86)	196.6	(334.88)	333.5
I_c		(253.40)	252.8	(345.33)	344.6

^a Results of r_α -refinements (the distances given are r_a -values). Distances, r_a , amplitudes, l , in Ångströms; angles in degrees; moment of inertia, I , in $u \text{ \AA}^2$. ^b See Fig. 3 for numbering of the atoms. ^c Parenthesized values are standard deviations obtained from the least-squares refinement (σ_{LS}) and they refer to the last digits given. For the distance parameters they should be corrected for systematic uncertainties according to $\sigma = [\sigma_{LS}^2 + (0.001 r)^2]^{\frac{1}{2}}$. Quantities in brackets are assumed values and primed amplitudes are refined in groups. ^d Agreement factor $R_w = [\sum w_i \Delta_i^2 / \sum w_i I_i^2(\text{obs})]^{\frac{1}{2}}$ where $\Delta_i = I_i(\text{obs}) - I_i(\text{th})$. ^e Moments of inertia (r_α -values); parenthesized values are microwave results (r_z -values). See text for estimates of uncertainties.

of the C—Cl bond out of the plane) did not reduce these problems, and such models were therefore discarded. The elements of the correlation matrices for the final refinements are given in Tables 5 and 6, respectively. The differences between the experimental and theoretical intensities and radial distribution curves calculated according to the final results given in Table 4, are shown in Figs. 1–4.

The r_a -values given in Table 4 were transformed to the corresponding r_α -values using the D -values of Table 3. The moments of inertia were calculated according to these values and the results are given in Table 4. The program employed, did not estimate the standard deviations in the calculated moments. However, increments of about 0.2 % to the distance

parameters (the standard deviation due to systematic uncertainties in the electron wavelength is usually estimated to 0.1 %) caused changes in the moments of inertia of about 0.4 %. Changes in the parameter values according to the standard deviations obtained from the least-squares procedure revealed, however, that the error limits for *cis*-chlorobutenyne should be at least 1 %, while 0.5 % should be a corresponding estimate for *trans*-chlorobutenyne.

DISCUSSION

The agreement factors given in Table 4 and the difference curves shown in Figs. 1–4

Table 5. Correlation matrix for parameters of *cis*-1-chlorobutenyne.

$r_{C\equiv C}$	r_{C-C}	$r_{C=C}$	$\angle C=C-C$	$\angle C=C-C$	r_{CH}	r_{C-Cl}	$\angle C=C-Cl$	$\angle C=C_1-H$	l_{ClC_1}	l_{C_1Cl}	l_{C_2Cl}	l_{C_3Cl}	l_{C-Cl}	Scale
														48 cm
														28 cm
1.0														
-0.03	1.0													
0.59	-0.16	1.0												
0.12	-0.28	0.06	1.0											
0.24	-0.09	0.16	0.55	1.0										
0.53	-0.02	0.47	0.06	0.18	1.0									
-0.04	0.02	-0.10	0.24	0.07	0.01	1.0								
-0.43	0.08	-0.55	-0.56	-0.26	-0.30	-0.33	1.0							
-0.13	-0.09	-0.06	0.60	0.28	-0.19	0.15	-0.35	1.0						
-0.17	-0.01	-0.16	0.06	0.00	-0.23	0.02	0.03	0.21	1.0					
0.08	0.00	0.06	-0.05	-0.10	-0.19	0.05	-0.01	-0.02	0.32	1.0				
-0.17	0.02	-0.09	-0.01	-0.15	-0.23	-0.04	-0.03	-0.14	-0.01	-0.14	1.0			
-0.26	-0.02	-0.10	-0.20	-0.16	-0.36	-0.07	0.21	0.03	0.22	0.06	0.21	1.0		
-0.47	0.11	-0.34	-0.15	-0.18	-0.54	-0.07	0.31	0.12	0.14	-0.04	0.30	0.52	1.0	
-0.34	0.10	0.18	-0.29	-0.23	-0.43	-0.14	0.29	0.00	0.20	0.02	0.35	0.67	0.48	1.0

demonstrate that the final structures are in fair agreement with the experimental data. The refined amplitude of vibration agree well with those calculated from the assumed force field (*cf.* Tables 3 and 4), and the moments of inertia obtained from the electron diffraction data are as compared to the estimated error limits in reasonable agreement with the microwave results.^{7,8} The model for *cis*-chlorobutenyne where a linear $C\equiv C-C$ chain was assumed, yielded moments of inertia in an overall poorer agreement with the microwave values.

The carbon-chlorine bond lengths are found to be 1.716(5) and 1.717(4) Å, respectively, for the *cis*- and *trans*-configuration; the parenthesized values correspond to 2σ where σ is corrected for systematic uncertainties (*cf.* Table 4, comment c). These are both in agreement with the $C(sp^2)-Cl$ bonds found in tetrachloroethylene⁹ (1.718(3) Å) and in *cis*-1,2-dichloroethylene¹⁰ (1.718(7) Å), while they seem to differ significantly from the corresponding bond in the monosubstituted ethylene where this bond is found to be 1.728(7) Å.¹¹ The $C=C-Cl$ angles in *cis*- and *trans*-1-chlorobutenyne are found to be 123.9(0.6) and 121.1(0.8)° and they confirm respectively to the $C=C-Cl$ angles in *cis*-dichloroethylene (123.8(0.5)°)¹⁰ and chloroethylene (121.1(0.9)°).¹¹ This correspondence seems reasonable as the environment with respect to steric strain should be quite similar in each pair of molecules. Differences in steric environment for the $C=C-C$ angles in *cis*- and *trans*-chlorobutenyne may also be used to account for the observed difference in this angle for the two compounds (123.9(0.6)° and 120.7(1.0)°, respectively). However, the $C=C-C$ angle in the unsubstituted hydrocarbon⁶ is 123.1(0.5)°, and the explanation for the decrease in this angle by chlorine substitution in the *trans* position appears far less obvious. The $C\equiv C-C$ chain in butenyne appears to be slightly bent⁶ ($\angle C\equiv C-C = 177.9(1.2)^\circ$). Significant deviations from linearity are, however, not observed in *cis*- and *trans*-1-chlorobutenyne (178.0(2.2)° and 180.2(2.4)°, respectively) although one might argue that there is a similar trend in the *cis*-compound. The $C-C$ bond distances in the two chlorobutenynes deviate slightly in a non-systematic manner from those in butenyne ($C\equiv C = 1.215(3)$ Å, $C=C = 1.344(4)$ Å, $C-C = 1.434(3)$ Å),

Table 6. Correlation matrix for parameters of *trans*-1-chlorobutenyne.

$r_{C\equiv C}$	r_{C-C}	$r_{C=C}$	$\angle C=C-C$	$\angle C=C-C$	r_{CH}	$\angle C=C_1-H$	r_{C-Cl}	$\angle C=C-Cl$
1.0								
0.16	1.0							
0.48	-0.14	1.0						
0.04	-0.49	-0.07	1.0					
0.62	-0.04	0.28	0.64	1.0				
0.34	-0.12	0.48	-0.04	0.20	1.0			
0.16	0.01	0.08	0.63	0.57	-0.14	1.0		
-0.16	0.00	-0.06	-0.12	-0.11	0.00	-0.01	1.0	
-0.59	-0.29	-0.58	-0.11	-0.50	-0.17	-0.54	-0.22	1.0
-0.77	-0.11	-0.21	-0.11	-0.50	-0.22	-0.15	0.17	0.39
0.18	0.48	-0.21	-0.22	0.00	-0.37	0.12	-0.07	-0.18
-0.04	0.14	-0.15	-0.06	-0.05	-0.17	0.00	-0.03	0.03
0.29	0.09	0.20	-0.37	-0.04	0.31	-0.43	-0.32	0.11
-0.06	0.13	-0.14	0.03	-0.01	-0.25	0.14	-0.07	-0.02
-0.08	0.08	-0.17	0.01	-0.04	-0.31	0.11	-0.04	0.02
-0.07	-0.03	-0.12	0.15	0.04	-0.38	0.23	-0.05	-0.01
-0.29	0.20	-0.33	0.00	-0.16	-0.53	0.20	-0.05	0.08
-0.06	0.19	-0.25	0.06	0.00	-0.48	0.26	-0.12	-0.03
l_{CH}	$l_{C_1C_1}$	$l_{C_1C_2}$	$l_{C_2C_1}$	$l_{C_2C_1}$	l_{C_1Cl}	l_{CCl}	Scales	
1.0							48 cm	28 cm
-0.21	1.0							
0.04	0.25	1.0						
-0.22	-0.05	-0.02	1.0					
0.04	0.33	0.11	-0.11	1.0				
0.00	0.28	0.14	-0.16	0.26	1.0			
0.00	0.32	0.20	-0.31	0.37	0.28	1.0		
0.21	0.43	0.16	-0.25	0.34	0.38	0.49	1.0	
-0.03	0.61	0.29	-0.22	0.51	0.46	0.65	0.54	1.0

while there seems to be a significant trend towards longer bond distances in the *trans*-isomer as compared to *cis*-chlorobutenyne. A discussion of the carbon skeleton in mono-chloro-substituted butenyne will be given and related to the unsubstituted butenyne in more detail in the last paper in this series.

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