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Vibrational spectra and force constants of *N*,*N*-dichloroacetamide and *N*-chloroacetamide

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Abstract—The i.r. and Raman spectra of *N*,*N*-dichloroacetamide and *N*-chloroacetamide are reported. The observed fundamental vibrations have been assigned on the basis of C_s symmetry. The frequencies corresponding to the N—Cl stretching modes were found below 500 cm^{-1}. In contrast they have been observed at much higher frequencies in pyramidal molecules. Normal coordinate analyses confirm the description of the fundamental vibrations; force constants were found to be transferable between molecules with related structures.

INTRODUCTION

VIBRATIONAL analyses of acetamide and some of its derivatives have been carried out previously [1–5]. A partial vibrational assignment of *N*-chloroacetamide has been reported [6] but no prevoius spectroscopic study of *N*,*N*-dichloroacetamide [7] has been discussed.

In an effort to understand the dynamics of these molecules and test the transferability of force constants among compounds with similar structures, the investigation of the infrared and Raman spectra of *N*,*N*-dichloroacetamide and *N*-chloroacetamide was undertaken. The Urey–Bradley potential function was used in the normal coordinate analysis.

EXPERIMENTAL

N,*N*-Dichloroacetamide was prepared as follows: acetamide (20 g) was dissolved in 200 ml of water and 20 g of sodium hydroxide added to the solution. Chlorine was bubbled through the cold (0–5°C) solution. A yellow-green oil was deposited in the bottom of the flask. The chlorine flow was stopped when no more oil was formed. The oil was separated from the aqueous solution and washed successively with two 50 ml portions of 20% aqueous sulfuric acid and two 50 ml portions of water. The crude *N*,*N*-dichloroacetamide (32 g; 70–75% yield based on acetamide, several runs), a yellow-green oil with a sharp odor, was then placed in a rotatory vacuum evaporator to remove the last traces of water. This product was further purified by trap to trap distillation in a vacuum line. Iodometric analysis indicated a purity greater than 99%. (Note: Although we did not encounter difficulty with these compounds, *N*,*N*-dichloroacetamide has been reported to detonate without apparent reason [7].)

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* Extracted in part from the doctoral dissertation of J. E. D. submitted to the Graduate School, University of Pittsburgh.

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N-chloroacetamide was prepared by the reaction of acetamide and chlorine in the presence of sodium bicarbonate [8], and recrystallized several times from chloroform, m.p. 109–110°.

Infrared spectra of *N*,*N*-dichloroacetamide were recorded from 4000 to 400 cm^{-1} in the gas phase, using a cell with KBr windows and 75 mm path; and from 4000 to 800 cm^{-1} in CCl_4 solution using a 0.05 mm path cell with NaCl windows. The i.r. spectra of *N*-chloroacetamide were obtained in KBr pellets and in $CHCl_3$ solution. Beckman IR-10 and IR-12 spectrophotometers were used in the measurements.

Raman spectra of *N*,*N*-dichloroacetamide as a pure liquid and of *N*-chloroacetamide in CH_3CN solutions were obtained with a Spex-Ramalog spectrophotometer exciting with the 6328 Å line of a Spectra-Physics Model 125 He–Ne laser. For the Raman spectra of solid *N*-chloroacetamide and its methanol solution the 4880 Å line of an argon ion laser was used. Polarization measurements were obtained by the usual two exposure method using a Polaroid disk.

Frequencies are believed to be accurate to ±1 cm^{-1} in the i.r. and ±2 cm^{-1} in the Raman spectra unless they appeared as broad or weak bands.

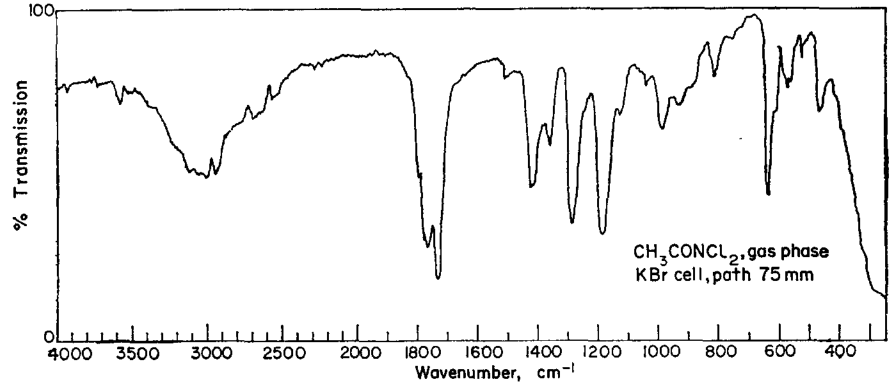

Fig. 1. Infrared spectrum of *N*,*N*-dichloroacetamide

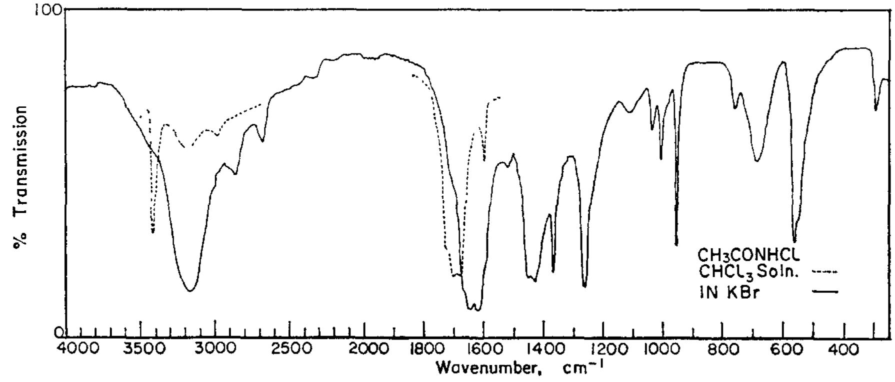

Fig. 2. Infrared spectrum of *N*-chloroacetamide

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VIBRATIONAL ASSIGNMENTS

Assuming C_s symmetry *N*,*N*-dichloroacetamide and *N*-chloroacetamide each have twenty-one fundamentals, $14a' + 7a''$. The i.r. spectra are shown in Figs. 1 and 2. The observed fundamental vibrations with the respective assignments are given in Tables 1 and 2.

Table 1. Observed frequencies (cm^{-1}) and assignments of *N*,*N*-dichloroacetamide

Infrared vapor	Infrared CCl_4 soln.	Raman* liquid	Assignment
a' Species			
		2936(13)P	CH_3 antisym. stretch
		2857(1)P	CH_3 sym. stretch
1772 1734 vs	1742 1715 vs	1724(11)P	C=O stretch
1427 s	1425 s	1433(7)P	CH_3 antisym. deform.
1372 m	1362 vs		CH_3 sym. deform.
1293 s	1289 s		CN stretch
1191 s	1192 vs	1194(4)P	CC stretch
1001 m	994 s	1002(17)P	CH_3 rock
830 w	827 w	837(9)P	C=O in-plane bend
596 582 w		596(85)P	CCN bend
478 m		468(100)P	NCl_2 antisym. stretch
		397(69)P	NCl_2 sym. stretch
		238(11)P	NCl_2 bend
		201(.5)	NCl_2 rock
a'' Species			
		3001(1)DP	CH_3 antisym. stretch
1033 w	1035 s		CH_3 rock
652 s			C=O wag
		284(37)DP	NCl_2 wag

* With He–Ne laser.
w, m, s: weak, medium, strong; v: very; P, DP: polarized, depolarized.

The hydrogen-bonded N—H stretching vibration of $CH_3CONHCl$ appears as a broad intense band around 3170 cm^{-1} in the i.r. spectrum of a solid sample. It is shifted to 3416 cm^{-1} in the i.r. spectrum of chloroform solution.

Each molecule has three methyl stretching vibrations, two of which belong to species a' and give rise to polarized Raman lines. They are observed in the Raman spectrum of liquid CH_3CONCl_2. However, in the Raman spectrum of an acetonitrile solution of $CH_3CONHCl$, only two weak bands are observed in the 3000 cm^{-1} region. The observed band in the 3000 cm^{-1} region of *N*,*N*-dichloroacetamide is unusually broad and poorly resolved. It is probable that several combination bands occur in this region in addition to the methyl stretching frequencies, thus accounting for the apparent complexity of the band.

The carbonyl stretching frequency (Amide I) can be unambiguously assigned to the polarized Raman line near 1700 cm^{-1} for both molecules.

In monosubstituted amides, [9], the N—H in-plane bending vibration has been observed at 1550 cm^{-1}. In $CH_3CONHCl$ a weak absorption band at 1597 cm^{-1} observed in solution is assigned to this mode (Amide II).

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[9] T. MIYAZAWA, T. SHIMANOUCHI and S. MIZUSHIMA, *J. Chem. Phys.* **24**, 408 (1956).

Table 2. Observed frequencies (cm^{-1}) and assignments of *N*-chloroacetamide

Infrared		Raman		
KBr pellet	$CHCl_3$ soln.	Solid*	Soln.	Assignment
a′ Species				
3170 s, b	3416 s			NH stretch
			2869(17)†	CH_3 sym. stretch
1653 1621 vs, b	1708 1677 vs	1650(93)	1712(23)P†	C═O stretch
	1597 w			CNH bend
1428 s				CH_3 antisym. deform.
1366 s		1365(7)		CH_3 sym. deform.
1263 s		1284(61)	1276(54)P‡	CN stretch
1007 m		1013(36)		CH_3 rock
955 s		965(95)	962(83)P‡	C—C stretch
		829(73)	829(43)P‡	C═O in-plane bend
568 557 s		596(100)	595(87)P†	CCN bend
		395(66)	394(100)P‡	NCl stretch
		244(45)	244(16)P‡	CNCl bend
			3002(28)†	CH_3 antisym. stretch
a″ Species				
1449 s		1443(12)	1439(49)DP†	CH_3 antisym. deform.
1036 w				CH_3 rock
763 w				N—H wag
693 m				C═O wag
304 w		300(50)		N—Cl out-of-plane bend

* Ar^+ laser. † He–Ne laser, in CH_3CN. ‡ Ar^+ laser, in MeOH.
w, m, s: weak, medium, strong; v: very; b: broad; P, DP: polarized, depolarized.

The assignment of the CH_3 deformations can be made by using previous assignments for the methyl group. In species *a′*, the antisymmetric deformation is found at 1427 and 1428 cm^{-1}, and the symmetric deformation at 1372 and 1366 cm^{-1} in CH_3CONCl_2 and $CH_3CONHCl$, respectively.

The CH_3 rocking fundamentals of the methyl group in acetamide [1, 2] and *N*-methylacetamide [3, 4] have been observed at about 1000 cm^{-1}. Accordingly, in CH_3CONCl_2 i.r. bands at 1001 and 1033 cm^{-1} are assigned to the *a′* and *a″* rocking vibrations, respectively. In $CH_3CONHCl$ the corresponding absorption bands occur at 1007 and 1036 cm^{-1}.

The CN stretching modes correspond to the strong absorption bands at 1293 and 1263 cm^{-1} in CH_3CONCl_2 and $CH_3CONHCl$, respectively. This assignment agrees with that of *N*-methylacetamide [3, 4] at 1296 cm^{-1}. In acetamide [1, 2] the corresponding fundamental is found at 1404 cm^{-1}. The C—C stretching vibration is observed in CH_3CONCl_2 at 1191 cm^{-1}, and in $CH_3CONHCl$ this mode appears at 955 cm^{-1}. A similar change in frequency has been observed in acetamide and *N*-methylacetamide where the frequencies are 874 and 1096 cm^{-1}, respectively.

Amides exhibit the C═O in-plane bending vibration (Amide IV) in the region 500–800 cm^{-1} [1, 9]. This fundamental is assigned to polarized Raman lines at 830 and 829 cm^{-1} in CH_3CONCl_2 and $CH_3CONHCl$, respectively. The CCN bending mode is assigned to polarized Raman lines at 595 cm^{-1} for both molecules.

The C═O wagging motion for amides has been assigned to a band in the region 600–800 cm^{-1}, depending on the physical state of the sample [9]. Thus, absorption bands observed at 652 and 693 cm^{-1} can be assigned to the C═O out-of-plane bending

Table 3. Symmetry coordinates for *N*,*N*-dichloroacetamide

a' Species	Description
$S_1 = \Delta r_{13}$	C—N stretch
$S_2 = \Delta r_{12}$	C—C stretch
$S_3 = \Delta r_{16}$	C=O stretch
$S_4 = (2\Delta\alpha_{435} - \Delta\alpha_{134} - \Delta\alpha_{135})/\sqrt{6}$	NCl_2 bend
$S_5 = (\Delta\alpha_{134} - \Delta\alpha_{135})/\sqrt{2}$	NCl_2 rock
$S_6 = (2\Delta\alpha_{316} - \Delta\alpha_{213} - \Delta\alpha_{216})/\sqrt{6}$	NCO bend
$S_7 = (\Delta\alpha_{213} - \Delta\alpha_{216})/\sqrt{2}$	CCN bend
$S_8 = (\Delta\alpha_{127} + \Delta\alpha_{128} + \Delta\alpha_{129} - \Delta\alpha_{728}$ $- \Delta\alpha_{729} - \Delta\alpha_{829})/\sqrt{6}$	CH_3 sym. deform.
$S_9 = (2\Delta\alpha_{829} - \Delta\alpha_{728} - \Delta\alpha_{729})/\sqrt{6}$	CH_3 antisym. deform.
$S_{10} = (2\Delta\alpha_{127} - \Delta\alpha_{128} - \Delta\alpha_{129})/\sqrt{6}$	CH_3 rock
$S_{11} = (\Delta r_{34} + \Delta r_{35})/\sqrt{2}$	NCl_2 sym. stretch
$S_{12} = (\Delta r_{34} - \Delta r_{35})/\sqrt{2}$	NCl_2 antisym. stretch
$S_{13} = (\Delta r_{27} + \Delta r_{28} + \Delta r_{29})/\sqrt{3}$	CH_3 sym. stretch
$S_{14} = (2\Delta r_{27} - \Delta r_{28} - \Delta r_{29})/\sqrt{6}$	CH_3 antisym. stretch
a'' Species	
$S_{15} = (\Delta r_{28} - \Delta r_{29})/\sqrt{2}$	CH_3 antisym. stretch
$S_{16} = (\Delta\alpha_{128} - \Delta\alpha_{129})/\sqrt{2}$	CH_3 rock
$S_{17} = (\Delta\alpha_{728} - \Delta\alpha_{729})/\sqrt{2}$	CH_3 antisym. deform.
$S_{18} = \Delta\pi$	C=O wag
$S_{19} = \Delta\theta$	NCl_2 wag
$S_{20} = \Delta\tau_{13}$	C—N torsion
$S_{21} = \Delta\tau_{12}$	C—C torsion

Table 4. Symmetry coordinates for *N*-chloroacetamide

a' Species	Description
$S_1 = \Delta r_{13}$	C—N stretch
$S_2 = \Delta r_{12}$	C—C stretch
$S_3 = \Delta r_{16}$	C=O stretch
$S_4 = (\Delta r_{27} + \Delta r_{28} + \Delta r_{29})/\sqrt{3}$	CH_3 sym. stretch
$S_5 = (2\Delta r_{27} - \Delta r_{28} - \Delta r_{29})/\sqrt{6}$	CH_3 antisym. stretch
$S_6 = \Delta r_{34}$	N—Cl stretch
$S_7 = \Delta r_{35}$	N—H stretch
$S_8 = (2\Delta\alpha_{316} - \Delta\alpha_{213} - \Delta\alpha_{216})/\sqrt{6}$	NCO bend
$S_9 = (\Delta\alpha_{213} - \Delta\alpha_{216})/\sqrt{2}$	CCN bend
$S_{10} = (2\Delta\alpha_{829} - \Delta\alpha_{728} - \Delta\alpha_{729})/\sqrt{6}$	CH_3 antisym. deform.
$S_{11} = (\Delta\alpha_{127} + \Delta\alpha_{128} + \alpha\Delta_{129} - \Delta\alpha_{728}$ $- \Delta\alpha_{729} - \Delta\alpha_{829})/\sqrt{6}$	CH_3 sym. deform.
$S_{12} = (2\Delta\alpha_{127} - \Delta\alpha_{128} - \Delta\alpha_{129})/\sqrt{6}$	CH_3 rock
$S_{13} = (2\Delta\alpha_{134} - \Delta\alpha_{435} - \Delta\alpha_{135})/\sqrt{6}$	CNCl bend
$S_{14} = (\Delta\alpha_{435} - \Delta\alpha_{135})/\sqrt{2}$	CNH bend
a'' Species	
$S_{15} = \Delta\tau_{13}$	N—Cl wag (CN torsion)
$S_{16} = (\Delta r_{28} - \Delta r_{29})/\sqrt{2}$	CH_3 antisym. stretch
$S_{17} = (\Delta\alpha_{128} - \Delta\alpha_{129})/\sqrt{2}$	CH_3 rock
$S_{18} = (\Delta\alpha_{728} - \Delta\alpha_{729})/\sqrt{2}$	CH_3 antisym. deform.
$S_{19} = \Delta\pi$	C=O wag
$S_{20} = \Delta\theta$	N—H wag
$S_{21} = \Delta\tau_{12}$	C—C torsion

mode for CH_3CONCl_2 and $CH_3CONHCl$, respectively. They were not observed in the Raman spectra.

In monosubstituted amides [9], the N—H wagging mode has been observed in the region around 750 cm^{-1}. The absorption band at 763 cm^{-1} can be assigned to this mode in $CH_3CONHCl$.

The NCl_2 antisymmetric and symmetric stretching modes in CH_3CONCl_2 are undoubtedly the strong polarized Raman lines at 469 and 397 cm^{-1}. The NCl_2 bending and wagging modes are assigned to bands at 238 and 284 cm^{-1} on the basis of polarization measurements. In $CH_3CONHCl$ the strong polarized Raman line at 394 cm^{-1} corresponds to the NCl stretch, while the polarized Raman line at 244 cm^{-1} can be assigned to the CNCl bending vibration. Precise determination of the structure of the molecules from Raman polarization measurements is precluded because of their low symmetry.

Excluding the torsional vibrations, two bands remain to be assigned in *N*,*N*-dichloroacetamide. They are the NCl_2 rocking vibration (a') which appears to be a very weak band observed in the Raman spectrum at 201 cm^{-1}, and the CH_3 antisymmetric deformation (a'') that was not observed.

In $CH_3CONHCl$, no assignment could be made for the CH_3 antisymmetric stretch, (a'), and the C—C torsion.

NORMAL COORDINATE CALCULATIONS

The normal coordinate treatments for *N*,*N*-dichloroacetamide and *N*-chloroacetamide were performed as 9-body problems using the model and molecular parameters

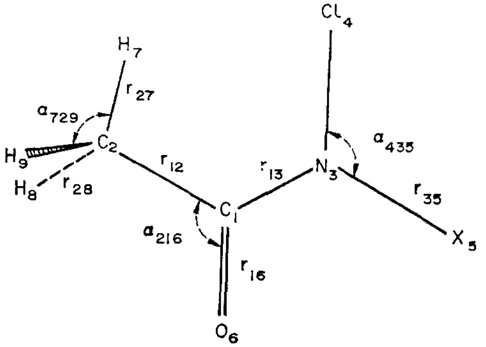

Fig. 3. Internal coordinates and molecular parameters for *N*,*N*-dichloroacetamide and *N*-chloroacetamide

X = Cl in *N*,*N*-dichloroacetamide, *X* = H in *N*-chloroacetamide.

Molecular parameters [12, 13]					
Bond distances (Å)		Angles (degrees)			
C—H	1.08	HCH	109.5	HCC	109.5
C—C	1.505	CCN	117.2	CCO	119.6
C—N	1.334	NCO	123.2	CNH	120
N—Cl	1.72	CNCl	120	ClNCl	120
N—H	1.02	HNCl	120		
C=O	1.26				

shown in Fig. 3. Structural parameters were assumed to be those found in an X-ray diffraction study of acetamide [10]. For the N—Cl bond distance a typical value of 1·72 Å, found in other molecules [11], was used. The potential function and the methods used were described previously by CARTER and DEVIA [12]. Coordinates for the torsion around the C—C and C—N bonds in CH_3CONCl_2 and around the C—C bond in $CH_3CONHCl$ were included in the calculation, but the force constants were not further adjusted because the corresponding frequencies were not observed. The internal tension constant (*k*) was given the value of −0.05 mdyn · Å found to give good results in other molecules containing a methyl group [1].

Most of the force constants shown in Table 5 fall into the ranges proposed by SHIMANOUCHI [13] and by SUSUKI [1] and were transferred directly to the calculation. They include stretching force constants for C—C, C—H and C=O, bending force constants for NC=O, CC=O, CCH and HCH, and repulsion force constants for CCH and HCH.

Table 5. Urey–Bradley force constants (mdyn/Å) for *N*,*N*-dichloroacetamide and *N*-chloroacetamide

	CH_3CONCl_2	$CH_3CONHCl$
K(C—C)	2.00	2.60
K(C—N)	4.50	3.80
K(C—H)	4.39	4.39
K(C=O)	9.87	8.80
K(N—Cl)	1.96	1.70
K(N—H)		5.84
H(HNCl)		0.20
H(ClNCl)	0.08	
H(CNCl)	0.11	0.18
H(NC=O)	0.37	0.37
H(CCN)	0.30	0.30
H(CC=O)	0.28	0.36
H(CCH)	0.24	0.24
H(HCH)	0.42	0.42
H(CNH)		0.42
P(C=O)*	0.71	0.57
P(NCl_2)*	0.16_3	
P(N—H)*		0.24_4
P(N—Cl)*		0.04
F(H. .Cl)		0.65
F(Cl. .Cl)	0.50	
F(C. .Cl)	0.93	0.60
F(O. .N)	1.80	1.80
F(O. .C)	0.60	0.80
F(C. .N)	0.71	0.71
F(CCH)	0.54	0.54
F(HCH)	0.03	0.03
F(CNH)		0.46
*k**	−0.05	−0.05

* mdyn · Å.

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[10] W. C. HAMILTON, *Acta Cryst.* **18,** 866 (1965).

[11] *Tables of Interatomic Distances and Configuration in Molecules and Ions,* The Chemical Society (1958); Supplement (1965).

[12] J. C. CARTER and J. E. DEVIA, *Spectrochim. Acta* **29A,** 623 (1973).

[13] T. SHIMANOUCHI, *Pure Appl. Chem.* **7,** 131 (1963).

DISCUSSION

According to Raman polarization measurements the equilibrium configurations of CH_3CONCl_2 and $CH_3CONHCl$ appear to have C_s symmetry. However, the model with no elements of symmetry, C_1, cannot be excluded because the observation of depolarized Raman bands does not indicate with certainty that they belong to non-totally symmetric vibrations. The agreement between observed and calculated frequencies obtained in the normal coordinate analyses is satisfactory on the basis of a simple Urey–Bradley force field approximation. The poor fit observed for the 1191 cm^{-1} band of CH_3CONCl_2 is attributed to the significant interaction between the CC bond and the methyl group, which is omitted in the UB model.

The values obtained for the force constants are in good agreement with those calculated for molecules with related structures [1, 13]. Some of the force constants were transferred directly and were not adjusted during the calculations to reduce the number of independent parameters.

The potential energy distribution among symmetry coordinates (Tables 6 and 7) confirms our approximate description of the fundamental frequencies and shows considerable mixing of the vibrational modes. The calculations also show that the CN and CC stretching modes in both molecules interact significantly, and are best described as the CCN antisymmetric and symmetric vibrations.

No significant differences were observed between the results of calculations for the two rotational isomers of *N*-chloroacetamide. The repulsion terms between oxygen–chlorine and oxygen–hydrogen are not taken into account in the UBFF potential energy expression, and the F matrix becomes common to both models. (The configuration with oxygen and chlorine on opposite sides of the CN bond was chosen as the most likely because of the minimum repulsion between the oxygen and chlorine atoms.)

Table 6. Observed and calculated frequencies (cm^{-1}) and potential energy distribution in *N*,*N*-dichloroacetamide

Observed	Calculated	PED
a' Species		
2936	2954	$S_{14}(100)$
2857	2868	$S_{13}(99)$
1753	1745	$S_1(12), S_3(89)$
1427	1438	$S_9(79), S_{10}(12)$
1372	1367	$S_1(15), S_8(82)$
1293	1299	$S_1(64), S_2(31), S_6(15), S_8(24)$
1191	1013	$S_1(20), S_2(11), S_6(10), S_{10}(38)$
1001	1022	$S_2(15), S_6(16), S_{10}(40)$
830	831	$S_2(30), S_5(16), S_{12}(55)$
582	590	$S_2(16), S_6(15), S_7(27), S_{11}(26)$
478	466	$S_6(22), S_{11}(22), S_{12}(37)$
397	391	$S_7(39), S_{11}(37)$
238	245	$S_4(85)$
201	191	$S_5(74), S_6(16), S_7(14)$
a'' Species		
3001	2954	$S_{15}(100)$
—	1441	$S_{16}(15), S_{17}(81)$
1033	1039	$S_{16}(85), S_{17}(18)$
652	651	$S_{18}(97)$
284	284	$S_{19}(100)$

Table 7. Observed and calculated frequencies (cm^{-1}) and potential energy distribution in *N*-chloroacetamide

Observed	Calculated	PED
a' Species		
3416	3415	$S_7(100)$
—	2955	$S_5(100)$
2869	2868	$S_4(99)$
1692	1710	$S_1(9)$, $S_3(52)$, $S_{14}(41)$
1597	1582	$S_3(37)$, $S_{14}(60)$
1428	1436	$S_{10}(80)$, $S_{12}(11)$
1366	1363	$S_{11}(100)$
1263	1289	$S_1(61)$, $S_2(44)$, $S_8(21)$
1007	1019	$S_{10}(12)$, $S_{12}(67)$
955	959	$S_1(32)$, $S_2(20)$, $S_6(14)$, $S_8(10)$, $S_{12}(10)$
829	776	$S_2(30)$, $S_6(26)$, $S_8(22)$, $S_{13}(16)$
563	555	$S_8(13)$, $S_9(60)$, $S_{13}(13)$
395	441	$S_6(65)$, $S_8(22)$
244	208	$S_8(12)$, $S_9(22)$, $S_{13}(64)$
a'' Species		
3002	2953	$S_{16}(100)$
1449	1441	$S_{17}(15)$, $S_{18}(81)$
1036	1039	$S_{17}(85)$, $S_{18}(18)$
763	763	$S_{20}(97)$
693	694	$S_{19}(96)$
304	307	$S_{15}(100)$

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