sulfate. Removal of the solvent followed by column chromatography (silica gel/benzene) gave 2-nitrohexan-5-one, 0.11 g (75% yield): IR (neat) 1720, 1545 cm^{-1}; NMR (CCl_4) δ 1.53 (d, 3 H), 2.09 (s, 3 H), 2.22-2.64 (m, 4 H), 4.2-4.6 (m, 1 H). Anal. Calcd for $C_6H_{11}NO_3$: C, 49.65; H, 7.64; N, 9.65. Found: C, 49.46; H, 7.92; N, 9.38.

Reaction of 5a with CH_3SNa. A mixture of **5a** (0.19 g, 1 mmol) and CH_3SNa (0.21 g, 3 mmol) in HMPA (10 mL) was stirred for 4 h at room temperature under nitrogen with exposure to a 150-W tungten lamp. GLC analyses revealed that no **5a** was left but **6c** was formed in 1% yield. The reaction mixture was worked up in the same way as the reaction of **1a** with CH_3SNa to give methyl thiobenzoate (0.11 g, 65% yield).

Reaction of 5c with CH_3SNa. A mixture of **5c** (0.18 g, 1 mmol) and CH_3SNa (0.21 g, 3 mmol) in HMPA (10 mL) was stirred for 72 h at room temperature under nitrogen with exposure to a 150-W tungsten lamp. GLC analyses revealed that **6c** was formed in 16% yield. After the same workup as employed in the reaction of **1a** with CH_3SNa, 0.14 g of **5c** was recovered.

Reaction of 5a with KOH in Ethylene Glycol. A mixture of **5a** (0.19 g, 1 mmol) and KOH (0.06 g, 1 mmol) in ethylene glycol (10 mL) was stirred for 4 h at 120 °C. The reaction mixture was poured into water and acidified with concentrates HCl to give benzoic acid (0.11 g, 89% yield).

Mechanistic Studies. Inhibition Experiments. The solutions containing **1a** (0.18 g, 1 mmol) and BNAH (0.64 g, 3 mmol) in DMF (10 mL) were prepared, into which a stream of nitrogen was passed. The first solution, the control, was irradiated by a 150-W tungsten lamp. The second solution also contained m-DNB (0.017 g, 0.1 mmol), and the third solution contained DTBN (0.02 g, 0.2 mmol); they were irradiated by a 150-W tungsten lamp. The amount of **2a** formed was measured by GLC after 6 or 17 h. Similar inhibition studies were also carried out using **5a** (1 mmol), BNAH (3 mmol), m-DNB (0.1 mmol), and DTBN (0.2 mmol). Results are summarized in Table IV.

Reduction of 1a by BNAH in the Presence of Sodium Dithionite. A mixture of **1a** (1.84 g, 10 mmol), BNAH (6.42 g, 30 mmol), and $Na_2S_2O_4$ (5.2 g, 30 mmol) in DMF (100 mL) was stirred for 2j h at room temperature under nitrogen in the dark. After the usual workup, column chromatography (silica gel/benzene) gave **2a** (0.42 g, 40% yield). The yield of **2a** was also determined by GLC.

Reaction of 1a with Sodium Dithionite. A mixture of **1a** (0.18 g, 1 mmol) and $Na_2S_2O_4$ (0.52 g, 3 mmol) in DMF (10 mL) was stirred for 24 h at room temperature. After the usual workup, the crude product was analyzed by GLC; no **2a** was detected.

Reduction of 1a by BNAH in the Presence of Di-*tert*-butyl Peroxyoxalate (DTPO). A mixture of **1a** (0.92 g, 5 mmol), BNAH (3.2 g, 15 mmol), and DTPO (0.94 g, 0.4 mmol), BNAH (3.2 g, 15 mmol), and DTPO (0.94 g, 0.4 mmol) in DMF (20 mL) was stirred for 24 h at room temperature under nitrogen in the dark. After the usual workup, column chromatography (silica gel/benzene) gave **2a** (0.82 g, 40% yield); GLC yield was 60%. At the same time a reaction carried out in the absence of DTPO gave no **2a**.

Reduction of 1a by BNAH in the Presence of AIBN. A mixture of **1a** (0.1, g, 1 mmol), BNAH (0.64 g, 3 mmol), and AIBN (0.016 g, 0.1 mmol) in DMF (10 mL) was heated at 80 °C for 3 h in the dark. The control did not contain AIBN. On workup the products were analyzed by GLC. Results are summarized in Table II.

Reduction of 1a by BNAH in CD_3CN. A mixture of **1a** (0.18 g, 1 mmol) and BNAH (0.64 g, 3 mmol) in CD_3CN (10 mL) was stirred for 24 h at room temperature under nitrogen with a exposure to a 150-W tungsten lamp. After the usual workup, column chromatography (silica gel/benzene) gave pure **2a** (0.07 g, 50% yield), in which deuterium was not contained. The content of deuterium was determined by NMR.

Reduction of 1a by 1-Benzyl-1,4-dihydronicotinamide-*4,4-d*$_2$. A mixture of **1a** (0.18 g, 1 mmole and 1-benzyl-**1,4**-dihydronicotinamide-**4,4-*d*$_2$** (D content is 85%, 0.65 g, 3 mmol) in CH_3CN (10 mL) was stirred for 24 h at room temperature under nitrogen with exposure to a 150-W tungsten lamp. After the usual workup, column chromatography (silica gel/benzene) gave the deuterated **2a**, whose D content was determined by NMR to be 65%.

Registry No. 1a, 74261-40-8; **1b**, 74261-41-9; **1c**, 74261-42-0; **2a**, 18397-63-2; **2b**, 74261-48-6; **2c**, 74261-49-7; **3a**, 74261-43-1; **3b**, 85422-78-2; **3c**, 85422-79-3; **4a**, 34927-40-7; **4b**, 10444-16-3; **4c**, 85422-80-6; **5a**, 29329-26-8; **5b**, 74261-44-2; **5c**, 14897-67-7; **5d**, 74261-45-3; **5e**, 74261-47-5; **5f**, 65662-59-1; **5g**, 74261-46-4; **6a**, 611-70-1; **6b**, 18713-58-1; **6c**, 93-55-0; **6d**, 6285-05-8; **6e**, 5337-93-9; **6f**, 121-97-1; **7**, 85422-81-7; CH_3SNa, 5188-07-8; $BNA^+NO_2^-$, 85422-82-8; BNAH, 952-92-1; 5-cyano-5-nitro-2-heptanol, 85422-83-9; 2-nitrohexan-5-one, 35223-72-4; 1-phenyl-2-methyl-2-nitropropanol, 33687-74-0; methyl 2-nitropropionate, 6118-50-9; acrylonitrile, 107-13-1; 2-nitrobutyronitrile, 85422-84-0; methyl vinyl ketone, 78-94-4.

Concerted Fragmentation of *N*-Chloro-α-amino Acid Anions

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Abstract: The decomposition of anions of *N*-chloro-α-amino acids in neutral aqueous solution gives chloride ion, imines (which hydrolyze rapidly to amine and carbonyl products), and carbon dioxide. The reactions are first order in the concentration of the *N*-chloro-α-amino acid anions and are independent of acidity between pH 5 and 9. The rate constants, which range from 4.2×10^{-6} s^{-1} to 9.0×10^{-2} s^{-1} at 25.0 °C, are highly dependent on the amino acid structure and values increase in the order: glycine < sarcosine < threonine < alanine < proline < α-aminoisobutyric acid < 1-amino-1-carboxycyclohexane. The factor of 21 000 in relative reactivity for this sequence, the large positive values found for $\Delta S^{\ddagger}$ (30-61 J K^{-1} mol^{-1}), and the products formed suggest that the reactions proceed by a concerted fragmentation mechanism.

N-Chloro-α-amino acids form rapidly in aqueous solution from the reaction of amino acids with chlorinating agents such as hypochlorous acid,[1-3] chlorine,[3] and monochloramine.[4,5] These reactions often occur when potable or waste waters are chlorinated for disinfection.[1,5] The *N*-chloro-α-amino acids are not stable and decompose to ammonia, chloride ion, carbon dioxide, and carbonyls.[2] The rate of decomposition of *N*-chloroalanine in water is first order in the chloroamino acid anion with a rate constant of 2.7×10^{-4} s^{-1} at 25.0 °C, independent of pH from 5 to 9.[6] The rate-determining step given in eq 1 is followed by the rapid hydrolysis of ethylimine (eq 2). Similar products have been reported when amino acids are brominated.[7]

$$ClNHCH(CH_3)CO_2^- \rightarrow Cl^- + HN{=}CHCH_3 + CO_2 \quad (1)$$

$$HN{=}CHCH_3 + H_2O \rightarrow NH_3 + O{=}CHCH_3 \quad (2)$$

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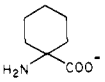
Table I. Rate Constants for the Decomposition of *N*-Chloro-α-amino Acid Anions in Aqueous Solution[a]

chloramine of	temp, °C	k_d, s^{-1}	relative k_d, 25 °C	$\Delta H^{\ddagger}$, kJ mol^{-1}	$\Delta S^{\ddagger}$, J K^{-1} mol^{-1}
Gly, $NH_2CH_2COO^-$	25.0	$4.2 (\pm 0.4) \times 10^{-6}$	1		
Sar, $CH_3NHCH_2COO^-$	14.9	$9.7 (\pm 0.8) \times 10^{-6}$			
	25.0	$5.07 (\pm 0.07) \times 10^{-5}$	12	115 (±2)	61 (±1)
	37.0	$3.43 (\pm 0.04) \times 10^{-4}$			
	46.1	$1.21 (\pm 0.02) \times 10^{-3}$			
Thr, $NH_2CH(CH(OH)CH_3)COO^-$	25.0	$2 (\pm 1) \times 10^{-4}$ [b]	50		
Ala, $NH_2CH(CH_3)COO^-$	6.0	$1.45 (\pm 0.07) \times 10^{-5}$			
	15.0	$6.4 (\pm 0.2) \times 10^{-5}$			
	25.0	$2.67 (\pm 0.02) \times 10^{-4}$	64	107 (±2)	45 (±1)
	37.0	$1.45 (\pm 0.04) \times 10^{-3}$			
Pro, 	25.0	$8.8 (\pm 0.2) \times 10^{-4}$	2100		
Aib, $NH_2C(CH_3)_2COO^-$	5.6	$7.8 (\pm 0.2) \times 10^{-4}$			
	13.6	$3.3 (\pm 0.4) \times 10^{-3}$			
	25.0	$1.29 (\pm 0.08) \times 10^{-2}$	3100	92 (±4)	30 (±2)
	37.0	$5.65 (\pm 0.09) \times 10^{-2}$			
Acc, 	25.0	$9.0 (\pm 0.1) \times 10^{-2}$	21000		

[a] pH 6.85, 0.01 M sodium phosphate buffer, 0.5 M ionic strength. [b] pH 7.15.

The mechanisms of these reactions have not been investigated in detail; however, the production of three molecules from a single reactant in eq 1 suggests that the mechanism of these decompositions may involve a simultaneous breaking of bonds in the transition state. Oxidative fragmentation of this type has been proposed in the reaction of hypochlorite with β-hydroxy amines.[8] The kinetics of decomposition of *N*-chloroethanolamine in strong base is attributed[9] to the fragmentation reaction of $ClNHCH_2CH_2O^-$.

Grob[10-12] has presented a unified characterization of concerted fragmentation reactions. An electron-withdrawing group, such as chlorine, and an electron-donating group, such as carboxylate, must be present in the same molecule for fragmentation to occur. When these groups are antiperiplanar to one another (Figure 1), then a facile fragmentation supersedes other decomposition pathways. The optimum conformation maximizes overlap of the p orbitals formed from the bonds of the leaving groups, facilitating electron flow and π-bonding. This mechanism has been studied in γ-amino chlorides[13] and in β-bromo acids.[14-17]

Becker and Grob[13] suggested that the decarboxylation of α-amino acids by hypochlorite is a possible fragmentation reaction and indicated that either *N*-haloamino acids or acyl hypohalides could be intermediates. The kinetics were not known. The present study shows that N-chlorination occurs first, followed by a first-order decomposition of the *N*-chloro-α-amino acid anion in aqueous solution. The reactions have large positive values of activation entropy, and the rates are highly dependent on the α-substituent groups. The products, the kinetics, the substituent effect, and the activation energy are all consistent with a concerted fragmentation mechanism.

Table II. Products of the Decomposition of *N*-Chloro-α-amino Acid Anions

N-chloramine of	carbonyl found[a]	% NH_3 found[a]
Gly	31 ± 3% formaldehyde <2% glyoxylic acid	74 ± 10
Sar	76 ± 3% formaldehyde 8 ± 2% glyoxylic acid	nd
Ala	100% acetaldehyde[b] <2% pyruvic acid	95 ± 13
Aib	99 ± 3% acetone	94 ± 12
Acc	95 ± 3% cyclohexanone	92 ± 13

[a] Expressed as a percentage of initial chloramine. [b] From ref 6. nd, not determined.

Experimental Section

Reagents. The amino acids α-aminoisobutyric acid (Aib) and alanine (Ala) were recrystallized from water; 1-amino-1-carboxycyclohexane (Acc) was recrystallized as the hydrochloride from 1 M HCl, glycine (Gly) from 50% ethanol, proline (Pro) from absolute ethanol, and sarcosine hydrochloride (Sar) from methanol. Threonine (Thr) was used as received. Chlorine was obtained from reagent grade sodium hypochlorite that had been standardized spectrophotometrically. The molar absorptivity of NaOCl is 350 M^{-1} cm^{-1} at 292 nm, based on iodimetry.[18]

The reactions were carried out in aqueous solution with the pH maintained at 6.85 with 0.01 M sodium phosphate buffer. Ionic strength was adjusted to 0.5 M with sodium perchlorate produced from the neutralization of Na_2CO_3 and $HClO_4$.

Procedures. Solutions of mono-*N*-chloro-α-amino acids (10^{-4}–10^{-3} M) were formed from a buffered solution of hypochlorous acid and a tenfold excess of the corresponding amino acid in buffer. The two solutions were always combined through a double twin-jet tangential mixer. Excess amine and efficient mixing impeded formation of dichloroamino acids. The formation of the chloroamino acid was always much faster than the subsequent decomposition.

The kinetics of decomposition were monitored at a convenient wavelength near the λ_{max} of the *N*-chloroamino acid (250–280 nm, $\epsilon \simeq 360$ M^{-1} cm^{-1})[3,4] either on a Cary 16 spectrophotometer or on a Durrum stopped-flow spectrophotometer interfaced to a Hewlett-Packard 2108B minicomputer.[19] Rate constants were determined from a slope of the least-squares linear regression of $\ln (A_t - A_\infty)$ vs. time where A_t is the absorbance at a specified time and A_∞ is the absorbance at the end of the reaction. Occasional deviations from linearity noted early in the reaction can be attributed to the decomposition of traces of dichloroamino acids, which are much more rapid to react.

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Table III. Comparison of Rate Constants for the Decomposition of Anions of *N*-Chloro-α-amino Acids and of β-Bromo Carboxylic Acids

chloramine of	k_d, s^{-1}	% fragmentation	corresponding β-bromo carboxylate[a]	k_d, s^{-1}	% fragmentation
Gly	4.2×10^{-6}	>31	β-bromopropionate	3.5×10^{-6}	0
Sar	5.1×10^{-5}	76	β-bromobutyrate	1.8×10^{-5}	15
Pro	8.8×10^{-3}	~100	*trans*-β-bromocyclopentanecarboxylate	4.5×10^{-4}	26

[a] From ref 27.

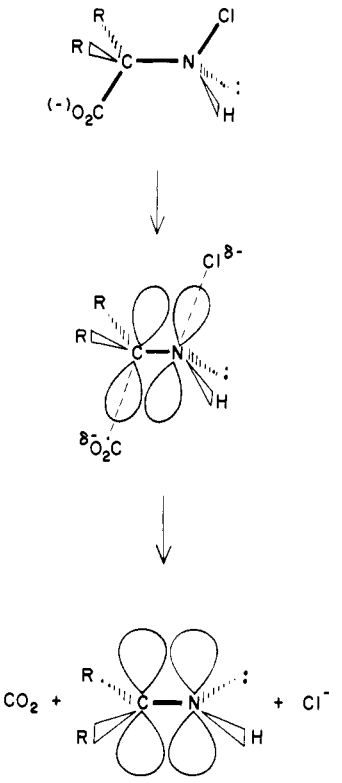

Figure 1. Transition from optimum antiperiplanar conformation of the *N*-chloro-α-amino acid anion to the π-bond in the imine product.

Ammonia was determined with an Orion ammonia-sensing electrode, Model 95-10. Formaldehyde was determined with the optimized chromotropic acid method.[20] A calibration curve was generated by dilution of a stock formaldehyde solution that had been assayed gravimetrically as the dimedone adduct.[20] The concentrations of other carbonyls were determined as their 2,4-dinitrophenylhydrazones, by using the spectrophotometric method of Wells.[21]

Results

Hypochlorous acid reacts rapidly with amino acids to form *N*-chloroamino acids. The *N*-chloro derivatives of β-amino acids and of peptides are much more stable in aqueous solution than are the *N*-chloro derivatives of α-amino acids.[3] The *N*-chloro derivative of each α-amino acid forms rapidly and undergoes a slower first-order decomposition reaction. The anion of the *N*-chloro-α-amino acid is the predominant form of this species present in solution, and the proposed rate-determining reaction is given in eq 1. First-order rate constants for *N*-Cl-Ala are independent of pH between 4.5 and 9.5. Changes in buffer composition (acetate, phosphate, borate), in buffer concentration (0–0.25 M), and in ionic strength have no appreciable effect on the rate constant.

The first-order rate constants for the decomposition are reported in Table I. These values change by more than 4 orders of magnitude for the *N*-chloroamino acids studied. The α-disubstituted compounds, *N*-Cl-Aib and *N*-Cl-Acc, decompose faster than the monosubstituted *N*-Cl-Ala, *N*-Cl-Thr, and *N*-Cl-pro, which are in turn faster than the unsubstituted *N*-Cl-Gly and *N*-Cl-Sar. Among compounds with the same number of substituents, larger substituents increase reactivity.

From the effect of temperature on the rate of decomposition (Table I), the enthalpy of activation is found to decrease as the reactivity of the compound increases. The entropy of activation decreases with increasing reactivity of the compound, but is large and positive in all cases.

Product determinations are summarized in Table II. The most reactive *N*-chloroamino acids produce the corresponding aldehyde or ketone and ammonia in nearly quantitative yield. In all cases the final products have no reactivity toward iodide; hence all the active chlorine is reduced to chloride. Those compounds with lower reactivity produce less of these products because of subsequent reactions of the products during the 10 days necessary for the slowest reaction to be completed. Previous workers[8] have reported difficulty in the isolation of formaldehyde due to its interaction with ammonia as well as its oxidation.

Discussion

The decomposition of *N*-chloro-α-amino acid anions proceeds primarily by a fragmentation mechanism. The observed first-order kinetics, independent of pH, are not consistent with a bimolecular mechanism, such as proton-assisted decarboxylation.[22] The more reactive *N*-chloro-α-amino acid anions give quantitative yields of the products expected from concerted fragmentation. Also concordant with a concerted fragmentation mechanism are the large observed changes in reaction rates with variation of substituents and the large positive entropies of activation.

The expected products from the reaction are fragments from the electron-donating group, the electron-withdrawing group, and an unsaturated compound.[12] For *N*-chloro-α-amino acid anions, these are CO_2, Cl^-, and an imine (eq 1); the imine hydrolyzes rapidly to ammonia and a carbonyl (eq 2). These products are recovered quantitatively from the decomposition of the more reactive chloramines of Ala, Aib, and Acc (Table II). Similar products would be expected from the chloroamines of Thr and Pro, which are as reactive as *N*-Cl-Ala (Table I). Quantitative recoveries of fragmentation products from the decomposition of acyclic compounds, as observed here, are unusual even for compounds that are generally thought to decompose by a fragmentation process.[11,23] The β-bromo carboxylates, which resemble *N*-chloro-α-amino acid anions in structure and in withdrawing and donating groups, produce a far lower percentage of fragmentation products than do the chloroamino acids (Table III). In fact, only the structurally rigid bicycle *trans*-10-bromo-9-carboxydecalin gives quantitative yields of CO_2 and olefin.[17] It is not unreasonable that the yields of ammonia and formaldehyde from the decomposition of *N*-Cl-Gly (Talbe II) are less than quantitative. Hydrolysis of *N*-Cl-Gly to hydroxyaminoacetic acid could compete with fragmentation. Deprotonation of the α-carbon atom, observed in alkaline solution,[6,24] might also compete with fragmentation, but then glyoxylic acid should be produced from *N*-Cl-Gly as well as from *N*-Cl-Sar (Table II), and it is not found in appreciable concentration.

The large changes in the rates of decomposition of the *N*-chloro-α-amino acid anions as the number and size of substituents is increased also suggest concerted fragmentation. We have observed that *N*-Cl-α-Ala decomposes far more rapidly than does *N*-Cl-β-Ala, which cannot fragment. The 12- to 21 000-fold increase in rate of decomposition for *N*-chloro-α-amino acids is of the same magnitude as the accelerations found in other fragmentation reactions. In the γ-amino chlorides[23] the rate of reaction

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is 20 to 10^6 times faster than for analogous chlorides that cannot fragment. Rates are enhanced by factors of 20 to more than 10^5 for cyclic β-bromo acids over a cyclic β-bromo acid that cannot achieve the antiperiplanar conformation.[17]

The large positive entropies of activation in the decomposition of *N*-chloro-α-amino acids are consistent with concerted fragmentation (Table I). Evidence from numerous reaction mechanisms in solution suggests that activation entropies of 30 J K^{-1} mol^{-1} or greater are consistent with a transition state that involves the breaking of more than one bond, such as would occur in concerted fragmentation.[25] Entropies of activation decrease as rate constants for *N*-chloro-α-amino acid decomposition increase. This may be due to decreased solvation of the larger, more hydrophobic molecules and the consequent decrease in the number of water molecules released as the carboxylate loses negative charge. (The degree of hydration of chlorine changes little as it gains negative charge, since substantial solvtion of the bonded chlorine is expected.)

No plausible intermediates can be proposed in place of one-step concerted fragmentation. The formation of a carbanion by spontaneous loss of CO_2[6] does not agree with the change in rate constant as a function of substituents because *N*-Cl-Gly would form the most stable carbanion and would be the most reactive rather than the least reactive species. A nitrenium ion[26] could be formed by loss of chloride, in analogy to the formation of a carbonium ion from certain γ-amino chlorides,[11] but such a species would be stabilized by electron-donating groups attached to the nitrogen. Hence *N*-Cl-Sar would decompose rapidly, contrary to fact. A nitrenium ion would also be expected to yield substitution and elimination products. Anchimerically assisted chlorine loss to form a four-membered oxazetidine ring similar to a β-lactone is also unlikely. A bond must be formed between the carboxylate oxygen and the nitrogen, and this bond must eventually be broken to produce the observed fragments. Such a bond formation is not in agreement with the large positive entropy of activation. Furthermore, intermediates of this type are quite unstable.[27,28]

The relative rates of decomposition of the various *N*-chloro-α-amino acid anions are largely determined by the ease with which the antiperiplanar conformation can be achieved; however, thermodynamic and steric effects also influence the trend. The disubstituted molecules are most likely to be in the antiperiplanar conformation and so are most likely to decompose readily. A conformer with the chlorine and carboxylate on opposite sides of the nitrogen–carbon bond is also favored by the interaction between the amine hydrogen and the carboxylate oxygen.[29]

The general grouping of the decomposition rates according to the number of substituent groups on the α-carbon is caused by thermodynamic effects. Highly substituted double bonds in olefins are more stable than less substituted ones.[30,31] and a similar trend probably holds for carbon-substituted imines. The transition states leading to substituted imines would then be more stable than those leading to similar compounds that are less substituted. As a result, the activation energies are lower and the rates are faster. In the *N*-chloro-α-amino acids, the rate constant increases by a factor of about 60 for each methyl group added to the α-carbon in the series *N*-Cl-Gly < *N*-Cl-Ala < *N*-Cl-Aib.

In addition to this thermodynamic effect and the conformational effect ascribed to fragmentation, steric effects also influence the relative reactivity of *N*-chloro-α-amino acid anions. Since the bond angles at the α-carbon and at the nitrogen must increase from 109° in the reactants to 120° in the product imines, factors that favor this change will accelerate the decomposition of the chloramine. For example, repulsion between the two methyl groups in *N*-Cl-Aib will tend to expand the bond angle at the α-carbon atom and decrease the energy required to reach the transition state. The two cyclic compounds, *N*-Cl-Pro and *N*-Cl-Acc, are particularly influenced by steric effects, though in opposite ways. The cyclic structure of *N*-Cl-Acc tends to restrict the opening of the bond angle between the two β-carbon atoms, but apparently the effects of fragmentation and thermodynamic stability affect the reactivity to a greater degree. By contrast the reactivity of *N*-Cl-Pro is enhanced by the decrease in eclipsing interactions on going from the five-membered saturated ring to the ring containing a double bond between carbon and nitrogen.

Conclusion

The rates of decomposition of seven *N*-chloro-α-amino acid anions show a difference in reactivity of greater than 4 orders of magnitude for small changes in substituent groups on the α-carbon. The difference is attributable to a combination of conformational, thermodynamic, and steric effects upon a concerted fragmentation mechanism. Unlike most acyclic systems, which decompose by fragmentation, *N*-chloro-α-amino acid anions yield fragmentation products quantitatively.

The amino acids most likely to be found in natural water, such as glycine,[32] produce the most stable chloroamine. Hence, *N*-chloro-α-amino acids may be a persistent form of active chlorine in chlorinated natural water systems.

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Registry No. *N*-Chloroglycine anion, 85507-53-5; *N*-chlorosarcosine anion, 85507-54-6; *N*-chlorothreonine anion, 85507-55-7; *N*-chloroaniline anion, 85507-56-8; *N*-chloroproline anion, 85507-57-9; *N*-chloro-α-aminoisobutyric acid anion, 85507-58-0; 1-(chloroamino)cyclohexanecarboxylic acid anion, 85507-59-1; glycine, 56-40-6; sarcosine, 107-97-1; threonine, 72-19-5; alanine, 56-41-7; proline, 147-85-3; α-aminoisobutyric acid, 62-57-7; 1-aminocyclohexanecarboxylic acid, 2756-85-6.

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