1684 © 1990 The Chemical Society of Japan Bull. Chem. Soc. Jpn., 63, 1684—1690 (1990) [Vol. 63, No. 6

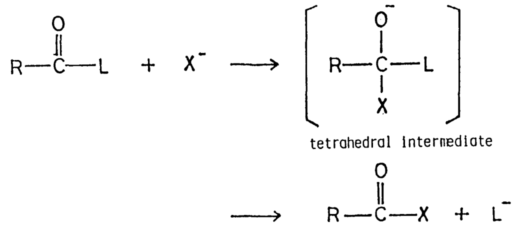
Dual Channels for Nucleophilic Displacements on Benzoyl Chlorides: Tetrahedral and Trigonal-Bipyramidal Transition States

Shinichi YAMABE,[*] Tetsuji KOYAMA, Tsutomu MINATO,[†] and Satoshi INAGAKI[††]
Department of Chemistry, Nara University of Education, Takabatake-cho, Nara 630
[†]Institute for Natural Science, Nara University, 1500 Misasagi-cho, Nara 631
[††]Department of Chemistry, Faculty of Engineering, Gifu University, Yanagido, Gifu 501-11

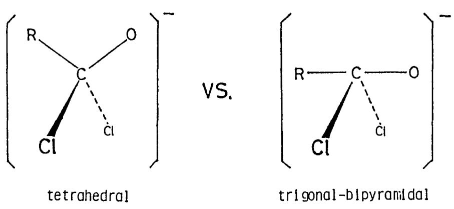
(Received October 26, 1989)

Nucleophilic substitutions on carbonyl carbons initiated by Cl^-, $Ph\text{-}CO\text{-}Cl + Cl^- \rightarrow Cl^- + Ph\text{-}CO\text{-}Cl$, were studied with ab initio MO calculations. Two transition states (TS's) were found. One is the "tetrahedral" TS caused by the π attack of the nucleophile. The other is the "trigonal-bipyramidal" TS initiated by the σ attack. The coexistence of two TS's is in accord with the proposals of Bentley and Cevasko et al. based on kinetic analyses. Two independent reaction paths are interpreted in terms of the frontier-orbital theory.

The bimolecular nucleophilic substitutions occur at carbonyl carbons. The reactions are believed to proceed via the stable tetrahedral intermediates, the addition-elimination mechanisms.[1)] L is a leaving group (nucleofuge) and X^- is a nucleophilic reagent.



Our previous computational work, however, suggested that the stable intermediate is not involved in the degenerated reaction (R=CH_3, X=L=Cl), $CH_3CO\text{-}Cl+Cl^-$.[2)] The middle point of the reaction process corresponds to the transition state (TS) like S_N2 reactions on the saturated carbons. A recent theoretical study supported our prediction, and two different TS geometries for the $Cl^-+RCO\text{-}Cl$ reaction (R=H) have been reported.[3)]



For R=Me, however, only the trigonal-bipyramidal TS has been found.[3)]

It is of mechanistic interest to analyze the electronic structures of these TS's, because the reason why they coexist in a reaction has not been elucidated yet. This work deals with the following two subjects on a more realistic reacting system, R=Ph, than small model systems investigated so far. One is the test of the basis-set dependence of TS geometries. The other is chemical justification of two TS's in a nucleophilic substitution.

Method of Calculation

The geometries of TS's were optimized with the ab initio MO calculations using the GAUSSIAN 82 program.[4)] The basis sets employed here were 3-21G, 3-21+(G), 4-31G, and 6-31G. The sign "+(G)" stands for the augumentation of the sp diffuse GTO[5)] only on the Cl atoms. The C_s symmetry was imposed on the TS-geometry optimization of $Cl^-+Ph\text{-}CO\text{-}Cl$. Whether the optimized geometry corresponds to TS should be examined through the vibrational analysis. However, the size of the present reacting system is too large to carry out directly the analysis, and an alternative model reacting system, $H_2C{=}CH\text{-}CO\text{-}Cl+Cl^-$, was employed for the analysis. With the 3-21G basis set, the tetrahedral TS geometry gives the sole imaginary frequency (=182i cm^{-1}). The trigonal-bipyramidal TS geometry also gives an imaginary one (=11i cm^{-1}). Although their absolute values are somewhat small as vibrational frequencies (due to the harmonic approximation), we may assign two geometries to saddle points. By analogy, two different stationary points with the C_s symmetry of $(Cl\cdots Ph\text{-}CO\cdots Cl)^-$ would correspond to two TS's. It appears to be somewhat doubtful to assign the trigonal-bipyramidal "TS" to a saddle point because of the small absolute value of the imaginary frequency. To check the position of the trigonal-bipyramidal "TS" on the potential energy surface, a full geometry optimization (without the C_s constraint) has been carried out, starting from the "TS" geometry. The resultant geometry is of a hydrogen-bonded system, $Cl^-\cdots H\text{-}C_6H_4\text{-}CO\text{-}Cl$. Thus, the trigonal-bipyramidal "TS" is not at an energy minimum but at a saddle point.

Since the system, $Cl^-+Ph\text{-}CO\text{-}Cl$, is large, the more detailed analysis of the basis-set dependence and the effect of the electron correlation than that in Table 1 is given in Appendix.

Results of Calculation

Table 1 shows TS geometries of the $Ph\text{-}CO\text{-}Cl+Cl^-$

S$_N$2 reaction with four basis sets. The present calculation gives two types of TS structures, tetrahedral and trigonal-bipyramidal, except the 4-31G basis set. The 4-31G basis set gives only the tetrahedral TS. The TS geometries with 3-21+(G) are shown in Fig. 1 together with that of the substrate.

The tetrahedral TS is discussed, first. The carbonyl C-O length, R1, is almost 1.2 Å, which shows that the double bond character is retained at TS. The C-Cl length, R3 is 2.2—2.3 Å, and that in TS of H-CO-Cl+Cl$^-$ is also calculated to be 2.2—2.3 Å with the four basis sets (not shown). Therefore, the length R3 is insensitive to the substituent R in the tetrahedral TS. The ∠PhCO angle A1 is 127—135°, which is somewhat basis-set dependent. The angle A1 at TS is larger than that (sp^2,≈120°) of the substrate, Ph-CO-Cl. A1 is found also to be slightly substituent-R dependent (i.e., for R=H, A1=133—142°). A1 depends on the electronic charge transferred from two chloride ions. The benzene ring is not distorted relative to the geometry of the substrate as Fig. 1 shows.

Second, the trigonal-bipyramidal TS is discussed. It is noteworthy that the C-O length R1 is smaller (≈1.115 Å) than that in the tetrahedral TS. The remarkably small R1 value is not of the carbonyl double bond, but is for the carbon monoxide (1.13 Å).

Table 1(a). TS Geometries and Energies of Benzoyl Chloride and Chloride Ion

Method	TS geometry$^{b)}$	Optimized parameters (C$_s$)						Total energy in a.u.
		R1$^{c)}$	R2$^{c)}$	R3$^{c)}$	A1$^{d)}$	A2$^{e)}$	B2$^{f)}$	
RHF/3-21G	T	1.167	1.481	2.305	133.0	100.0	130.1	−1255.59056
	T-B	1.115	1.413	3.199	180.0	99.1		−1255.59614
RHF/3-21+(G)$^{a)}$	T	1.163	1.480	2.334	135.3	99.7	129.3	−1255.61867
	T-B	1.116	1.408	3.317	180.0	98.6		−1255.63146
RHF/4-31G	T	1.191	1.491	2.185	126.8	102.5	129.3	−1260.38576
	T-B							
RHF/6-31G	T	1.180	1.486	2.260	129.9	102.2	129.3	−1261.69666
	T-B	1.116	1.417	3.283	180.0	98.5		−1261.69960

a) RHF/3-21+(G) data are also given in Fig. 1, and the "G" in the parenthesis denotes the addition of sp-type GTO on the chlorine atom. b) T and T-B stand for tetrahedral and trigonal-bipyramidal TS's, respectively. c) Bond distances in Å. d) Bond angles in degree. In the T-B TS, the C$_{2v}$ symmetry is obtained, that is, A1=180°. e) Bond angles in degree. f) Dihedral angles in degree.

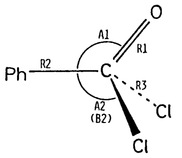


Table 1(b). TS Geometries (Phenyl Part) of Benzoyl Chloride and Chloride Ion

Method	TS geometry$^{b)}$	Optimized parameters (C$_s$)					
		R4$^{c)}$	R4′$^{c)}$	R5$^{c)}$	R5′$^{c)}$	R6$^{c)}$	R6′$^{c)}$
RHF/3-21G	T	1.381	1.382	1.386	1.378	1.380	1.390
	T-B	1.401		1.378		1.386	
RHF/3-21+(G)$^{a)}$	T	1.384	1.382	1.386	1.380	1.381	1.389
	T-B	1.401		1.378		1.387	
RHF/4-31G	T	1.382	1.384	1.386	1.378	1.379	1.388
	T-B						
RHF/6-31G	T	1.388	1.388	1.390	1.383	1.384	1.392
	T-B	1.405		1.382		1.390	

a) RHF/3-21+(G) data are also given in Fig. 1, and the "G" in the parenthesis of denotes the addition of sp-type GTO on the chlorine atom. b) T and T-B stand for tetrahedral and trigonal-bipyramidal TS's, respectively. c) Bond distances in Å. In the T-B TS, the C$_{2v}$ symmetry is obtained, that is, R4=R4′, R5=R5′, and R6=R6′.

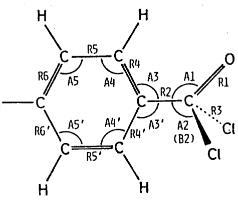
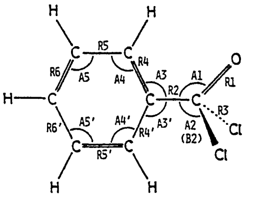
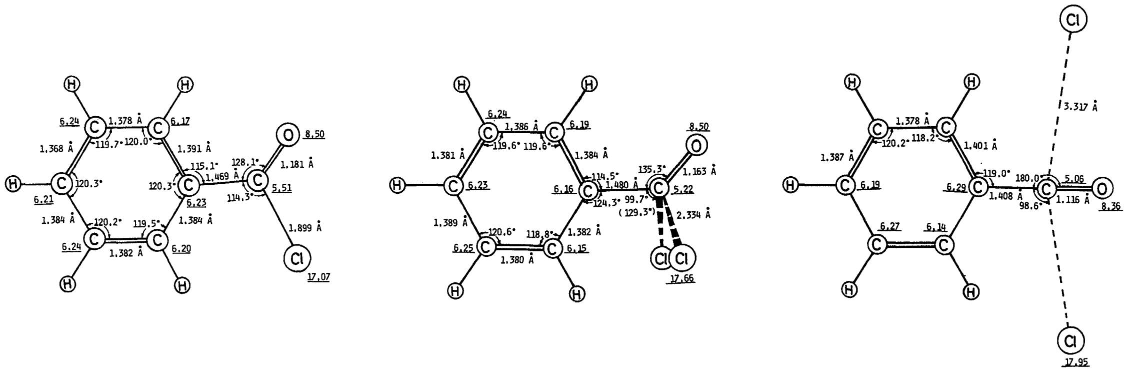


Table 1(c). TS Geometries (Phenyl Part) of Benzoyl Chloride and Chloride Ion

Method	TS geometry[b)]	Optimized parameters (C_s)					
		A3[c)]	A3′[c)]	A4[c)]	A4′[c)]	A5[c)]	A5′[c)]
RHF/3-21G	T	115.1	124.2	119.8	119.3	119.8	120.5
	T-B	119.0		118.3		120.3	
RHF/3-21+(G)[a)]	T	114.5	124.3	119.6	118.8	119.6	120.6
	T-B	119.0		118.2		120.2	
RHF/4-31G	T	116.6	123.6	120.2	119.9	119.9	120.4
	T-B						
RHF/6-31G	T	116.1	123.6	119.9	119.6	119.9	120.4
	T-B	119.0		118.2		120.3	

a) RHF/3-21+(G) data are also given in Fig. 1, and the "G" in the parenthesis denotes the addition of sp-type GTO on the chlorine atom. b) T and T-B stand for tetrahedral and trigonal-bipyramidal TS's, respectively. c) Bond angles in degree. In the T-B TS, the C_{2v} symmetry is obtained, that is, A3=A3′, A4=A4′, and A5=A5′.





Substrate Tetrahedral TS (C_s) Trigonal-Bipyramidal TS (C_{2v})

Fig. 1. 3-21+(G) Optimized Geometries of the Substrate and Two TS's for Ph-CO-Cl+Cl⁻. Geometric parameters are also given in Table 1. The number in parenthesis (129.3°) of the tetrahedral TS denotes the dihedral angle. Underlined numbers stand for atom electronic charges.

The C-C bond length, R2, is also smaller (≈1.41 Å) than that of the tetrahedral TS. This result indicates that the extent of the phenyl-carbonyl conjugation is larger in the trigonal-bipyramidal TS. The C···Cl distance R3 is 3.2—3.3 Å. Cl⁻ ions are almost isolated from the carbonyl carbon. R3 is substituent dependent, 2.6 Å at R=H, 2.9 Å at R=Me, and 3.3 Å at R=Ph with the 3-21+(G) basis set. This extraordinarily large distance must be related to the small C-O length, R1, and this relation will be discussed in the next Section. The benzene ring is deformed somewhat more than that in the tetrahedral TS, but the extent of the deformation is not so significant.

Total energies of two TS's are computed in Table 1(a). Except 4-31G, the trigonal-bipyramidal TS is more favorable than the tetrahedral TS. The former gets the stability of the ion-center separation as Fig. 1 shows.

Reviewing computed data in the Table, we may find out that the TS geometry does not depend on the basis set significantly except 4-31G. We may conclude that the reaction Ph-CO-Cl+Cl⁻ has two TS geometries.

Discussion on Two Reaction Channels. It is interesting that there are two independent TS's with common reactants and products. The coexistence is thought to stem from the fact that two frontier orbitals σ^*_{C-Cl} and π^*_{C-O} are available. In our previous work,[6)] the role of these orbitals on the tetrahedral TS was discussed in terms of the MO mixing. The tetrahedral TS is characterized by two semi-single C···Cl bonds plus a (σ single+two π semi-single) C-O bond. The TS is brought about by the out-of-plane geometric distortion of the substrate, acyl chloride. The distortion leads to the π*-σ* orbital mixing which is effective to the charge transfer from the nucleophile, Cl⁻, to the cationic carbonyl carbon. The carbonyl C=O length is kept invariant through the displacement reaction.[2] The π donative and $\bar{\pi}$ back-donative interactions work cooperatively to fix the C–O length.

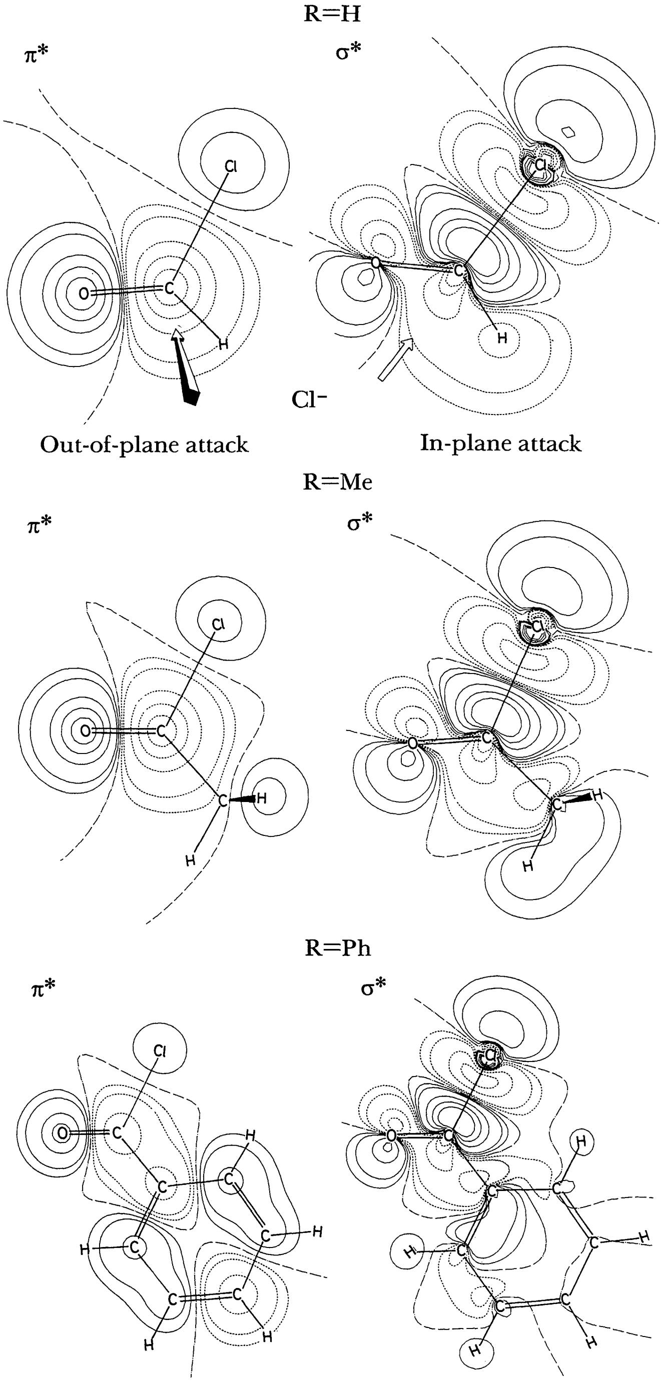
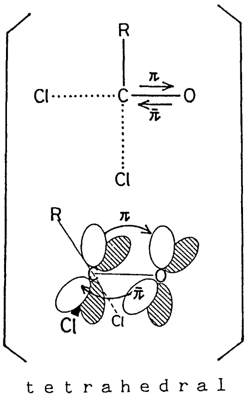
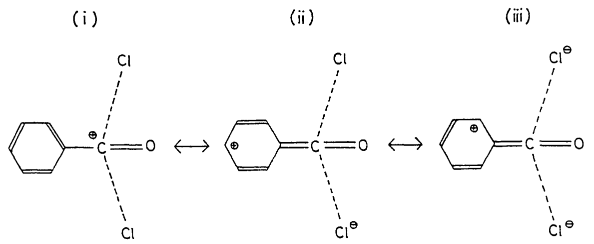


Fig. 2. Frontier vacant orbitals of formyl chloride (R=H), acetyl chloride (R=Me), and benzoyl chloride (R=Ph), for the nucleophilic attack (calculated by STO-3G basis set). π* MO's are drawn 0.5 Å above the molecular plane. The STO-3G orbital energies are 0.231 a.u. (π*) and 0.297 a.u. (σ*) for R=H, 0.244 a.u. (π*) and 0.293 a.u. (σ*) for R=Me, 0.173 a.u. (π*) and 0.306 a.u. (σ*) for R=Ph, respectively. For R=H, two routes of the Cl^- attack are shown by bold arrows.



The Cl^- attack to the π* MO on the carbonyl carbon leads to the tetrahedral TS.

The trigonal-bipyramidal TS is analyzed here. In view of the electron distribution (underlined numbers) in Fig. 1, the trigonal-bipyramidal TS is zwitterionic. The TS is represented as two chloride ions and Ph-C^+-O. This picture is reminiscent of S_N1 intermediates, i.e., the carbonium ion solvated by a reagent and a leaving group. In Table 1(a), the trigonal-bipyramidal TS is energetically more favorable than the tetrahedral TS. The superiority of the former may be attributed to the following resonance structures.



The reaction routes leading to the two TS's are investigated. At the initial stage of S_N2 reactions, the orientation of the nucleophilic Cl^- is determined by the shape of the frontier orbitals of the substrate. In Fig. 2, maps of these orbitals π* and σ* of the benzoyl chloride are drawn together with those of formyl (R=H) and acetyl (R=Me) chlorides. Comparison of these maps will inform us of the substituent effect on the reaction route. For the simplest substrate (R=H), two routes, i.e., π* and σ* attacks, are likely. For the acetyl chloride, however, the back side of the C–Cl bond is somewhat blocked by the methyl group. The slightly out-of-plane direction should be taken by nucleophiles. The trend is more remarkable in the benzoyl chloride. The ortho benzene proton sterically hinders the in-plane σ* attack.

Thus, in benzoyl chloride, it appears that the path leading to the trigonal-bipyramidal TS is narrow and unfavorable. The handicap for the trigonal-bipyramidal TS may be overcome by the geometric distortion through normal vibrational modes of substrate. Figure 3 gives a schematic presentation of two

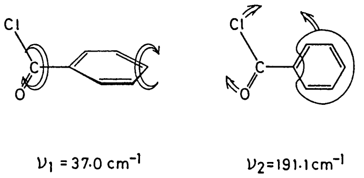
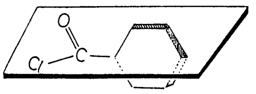


Fig. 3. Two vibrational modes of small frequencies of benzoyl chloride among 36 (3×14 atoms-6) modes by the STO-3G basis set.

vibrational modes of small frequencies. The ν_1 (=37.0 cm^{-1}) vibration is regarded almost as a free rotation around the C–C bond. In fact, the following out-of-plane substarate is only 3.9 kcal mol^{-1} (STO-3G) less stable than the planar molecule.



The rotation facilitates the reaction via the trigonal-bipyramidal TS. In addition, in-plane deformation of ν_2 (=191.1 cm^{-1}) spreads the route. Thus, the σ-attack becomes ready through the ν_1–ν_2 coupling given by the perturbation of the nucleophile. Besides the avoidance of the steric effect, the ν_1 rotation gives another favorable effect on the path. That is, in the out-of-plane geometry of benzoyl chloride, the $\sigma^*_{\mathrm{C-Cl}}$ MO mixes in phase with π^*_{ph} to give the new low-lying LUMO and consequently a better target of the nucleophile than that ($\sigma^*_{\mathrm{C-Cl}}$) of the planar substrate (Fig. 4).

The relation of two TS's is discussed. Whether a route connecting them is present or not is a mechanistic question. According to the different spatial directions of π* and σ* MO's, the in-plane and out-of-plane paths seem to be independent. That is, nucleophiles are fated to take either path, and their junction would be energetically high. The improbability of the interchange of two TS's is deduced by their entirely different geometries in Fig. 1. In the tetrahedral TS, two semi-single C···Cl bonds are present, while in the trigonal-bipyramidal TS they are absent. The change of the length of two bonds gives rise to a large energy barrier.

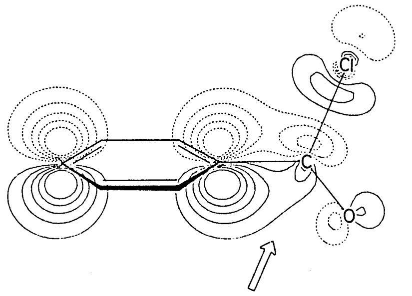
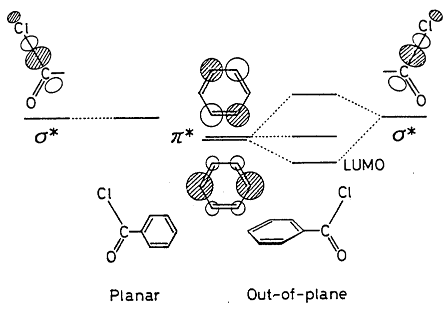
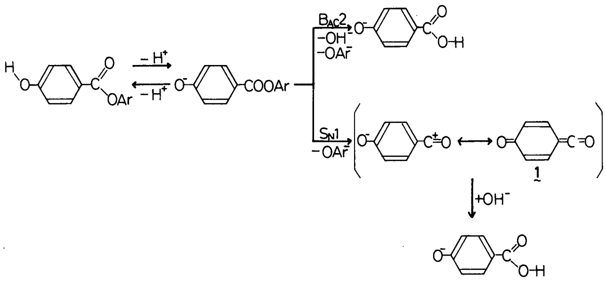


Fig. 4. Contour map of LUMO for the Distorted (out-of-plane) benzoyl chloride. This is "a better target".



Comparison with the Mechanistic Analysis Based on Kinetic Data. It is mechanistically surprising that two independent TS's are present with the common reactants and products for Cl$^-$+benzoyl chloride. If this is true, two reaction channels of the nucleophilic substitution on the unsaturated carbon should exist. This curious computed data must be compared with experimental evidence.

Cevasko et al.[7a] carried out a alkaline hydrolysis of aryl 4-hydroxybenzoates and proposed that there are associative ($\mathrm{B_{AC}2}$) and dissociative ($\mathrm{S_N1}$ or $\mathrm{E1_{CB}}$) paths. In the latter path, a ketene fused into the aromatic ring (like quinone) is considered as an $\mathrm{S_N1}$ intermediate, **1**.



$\mathrm{B_{AC}2}$ favored by poor leaving groups corresponds to the tetrahedral TS, and $\mathrm{S_N1}$ favored by good leaving groups to the trigonal-bipyramidal TS. In fact, Cevasko et al.[7b] deduced that the $\mathrm{B_{AC}2}$ TS geometry is tetrahedral and the bond interchange is synchronous. More importantly, they suggested that in the $\mathrm{S_N1}$ intermediate two bonds from carbonyl carbon to the nucleophile and to the leaving group have the zero strength. The *para* oxide anion stabilizes the intermediate through the fused-ketene resonance structure of **1**. Aside from this extra stabilizing effect, their suggestion is reasonably reflected in our computed geometry of Fig. 1. That is, in the trigonal-bipyramidal TS, two Cl ions are almost isolated from the ketene fused into the phenyl ring. Thus, the proposal of Cevasko et al. that two discrete paths should exist is consistent with our computed results.

Our mechanism is also in line with the experimental observation of Bentley and Koo.[8] They pointed out that there should be two simultaneous reaction channels for solvolysis of benzoyl chloride and *para*-methylbenzoyl chloride. Their postulate was based on the upward deviation from the Hammett-type plot in the slow-rate region. The kinetic data may be

TS	Route	Frontier orbital	Geometrical condition	Frequency factor, *A*	Activation energy, E_a
Tetrahedral	Out-of-plane	π^*	None	Large	Large
Trigonal-bipyramidal	In-plane	σ^*	Twisting	Small	Small

interpreted as follows. For a good nucleophile, the σ attack occurs predominantly. For a poor nucleophile, the π and the σ attacks take place simultaneously.

In view of the consistency with experimental evidence, we may say that the benzoyl carbon undergoes intrinsically two different modes of the nucleophilic attack.

Concluding Remarks

A nucleophilic substitution reaction on the unsaturated carbon of the benzoyl chloride has been investigated. Different from nucleophilic reactions on the saturated carbon, those on the unsaturated one are shown to have two independent routes (via S_N2-like tetrahedral TS and S_N1-like trigonal-bipyramidal TS). The presence of two routes is ascribed to the fact that there are two frontier orbitals σ^*_{C-Cl} and $\pi^*_{C=O}$ on the substrate. If X^- approaches the π^* MO, the tetrahedral TS is brought about through the σ^*-π^* MO mixing. The attack on the back side of the C-Cl bond in the molecular plane or its near region leads to trigonal-bipyramidal TS.

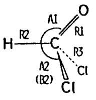
Energetically, this trigonal-bipyramidal TS is more favorable. However, the TS may be arrived at only through the distorted geometry of the substrate. That is, the twisting-mode vibration of the remarkably small frequency widens the back-side route of the C-Cl bond and lowers the energy level of the σ^* MO for the ready charge acceptance. Since the in-plane path becomes probable only for the sufficiently twisted substrate, the Arrhenius frequency factor would be much smaller than that of the out-of-plane path. The area of this path (π^* MO attack) is extremely large above and below the molecular plane for the large reaction probability. The characteristics of two TS's are compared in the above Table.

Solvent effect on TS energies is discussed. At the substrate geometry in Fig. 1, the carbonyl oxygen is anionic (8.50) and the protic solvent will be bonded to the oxygen atom. The formation of this hydrogen bond blocks the in-plane σ^* approach of the nucleophile, Cl^-. On the other hand, the out-of-plane π^* direction is almost free from the solvation and the large collisional frequency is probable also in the solution. The contrast in the hydrogen-bond formation between the blocked σ^* direction and the free π^* direction magnifies the difference of the frequency factor, *A*, in the above Table, (large, small)→(larger, smaller). Contrary to the solvent effect on *A*, the liquid-phase reactivity of the in-plane path becomes

Table 2. TS Geometries and Energies of Formyl Chloride and Chloride Ion

Method[a)]	TS geometry[b)]	Optimized parameters (C_s)						Total energy in a.u.
		R1[c)]	R2[c)]	R3[c)]	A1[d)]	A2[d)]	B2[e)]	
RHF/3-21G	T	not found						
	T-B	1.121	1.056	2.601	180.0	71.7		−1027.32653
RHF/3-21+G	T	1.176	1.060	2.242	138.3	91.3	128.9	−1027.36734
	T-B	1.121	1.058	2.620	180.0	71.6		−1027.36979
RHF/3-21+(G)	T	not found						
	T-B	1.118	1.058	2.635	180.0	71.6		−1027.35854
RHF/4-31G	T	1.183	1.062	2.179	133.2	93.6	129.0	−1031.15935
	T-B	1.125	1.054	2.551	180.0	70.6		−1031.15029
RHF/6-31G	T	1.170	1.060	2.256	138.8	90.9	128.2	−1032.22718
	T-B	1.122	1.060	2.629	180.0	70.7		−1032.23008
RHF/6-31+(G)	T	1.164	1.059	2.286	141.3	89.7	127.7	−1032.23574
	T-B	1.120	1.061	2.655	180.0	70.9		−1032.24122
MP2/3-21+(G)	T	1.195	1.073	2.359	141.6	89.5	126.2	−1027.69772
	T-B	1.160	1.068	2.643	180.0	73.7		−1027.69691

a) The "G" in the parenthesis of Method denotes the addition of sp-type GTO on the chlorine atom. b) T and T-B stand for tetrahedral and trigonal-bipyramidal TS's, respectively. The T-B geometry is calculated to be of C_{2v} symmetry. c) Bond distances in Å. d) Bond angles in degree. e) Dihedral angles in degree.



larger in terms of the activation energy, E_a. This is because the trigonal-bipyramidal TS is more zwitterionic and undergoes larger electrostatic stabilization than the tetrahedral TS. The difference of the extent of the solvation leads to the change of E_a in the Table, (large, small)→(larger, smaller). That is, through the solvation, the contrast in the Table becomes magnified.

Appendix

To check the quality of the calculated data in Table 1, a more detailed anaysis is made for a model (R=H) system, Cl^-+H-CO-Cl. With seven methods, the TS geometries are optimized and results are displayed in Table 2. Trend of the computed data in Table 2 is found to be similar to those in Table 1. For instance, in the T-B TS, all the methods give the short C-O (=1.12—1.16 Å) length. The C···Cl length is large (R3≃2.6 Å); that is, Cl^- is almost isolated from the carbonyl carbon.

A noticeable difference is found in two Tables. With RHF/3-21+(G), the tetrahedral TS is absent for R=H, whereas it is present for R=Ph. However, this difference is critical and method-dependent. In fact, with the MP2/3-21+(G) optimization, two TS's of almost same energies are obtained. The geometry of T-B TS calculated by MP2/3-21+(G) is quite similar to that calculated by RHF/3-21+(G), which indicates that the electron correlation does not alter the RHF geometry. Also, the electronic correlation is found to correct the overestimate of the stability of the RHF T-B TS. Through the improvement of the basis set, RHF/3-21+(G)→RHF/6-31+(G), also the T-B geometry is almost invariant.

The authors thank the Institute for Molecular Science for the allotment of the CPU time of the HITAC M-680H computer.

References

1) See, for instance, D. J. Cram and G. S. Hammond, "Organic Chemistry," 2nd Ed., McGraw-Hill, New York (1964), Chap. 17.

2) S. Yamabe and T. Minato, *J. Org. Chem.*, **26**, 2972 (1983).

3) J. F. Blake and W. L. Jorgensen, *J. Am. Chem. Soc.*, **109**, 3856 (1987).

4) GAUSSIAN82: J. S. Binkley, M. J. Frisch, D. J. Defrees, K. Raghavachari, R. A. Whiteside, H. B. Schlegel, and J. A. Pople, Carnegie-Mellon Chemistry Publishing Unit, Pittsburgh (1984).

5) T. Clark, J. Chandrasekhar, G. W. Spitznagel, and P. v. R. Schleyer, *J. Compt. Chem.*, **4**, 294 (1983).

6) S. Yamabe, T. Minato, and Y. Kawabata, *Can. J. Chem.*, **62**, 235 (1984).

7) a) G. Cevasco, G. Guanti, A. R. Hopkins, S. Thea, and A. Williams, *J. Org. Chem.*, **50**, 479 (1985). b) S. Thea, G. Cevasco, G. Guanti, N. Kashefi-Naini, and A. Williams, *ibid.*, **50**, 1867 (1985).

8) T. W. Bentley and I. S. Koo, *J. Chem. Soc., Chem. Commun.*, **1988**, 41.