Preparation of benzoyl fluoride from benzotrifluoride catalyzed by niobium oxide

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ABSTRACT

Several metals were found to catalyze the conversion of benzotrifluoride to benzoyl fluoride in the presence of carboxylic acids and sulfonic acids, together with the corresponding anhydride, and molecular oxygen. Nb_2O_5 exhibited the highest activity, and a conversion of ~99.8% and a selectivity of ~90% were obtained in 10 min under mild conditions. The composition of the acid and anhydride was found to play two roles – as a proton source to activate the C–F bond and as an oxygen transfer agent to form benzoyl fluoride. Oxygen facilitated fluorine transfer but did not enter into the reaction products. A possible mechanism for the conversion of benzotrifluoride to benzoyl fluoride was proposed.

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1. Introduction

Benzoyl fluoride has attracted recent interest as a precursor for a variety of pharmaceuticals and other organic products. For example, benzoyl fluoride can be used to make Rifamycins, antibiotics used to treat tuberculosis as well as exhibiting anti-tumor and anti-inflammatory activity [1]; to convert phosphoroazolides into phosophorofluorideates, potent enzymatic inhibitors [2]; and to acylate weakly basic aromatic amines to form analogs of the antitumor agent CC-1065 [3]. Benzoyl fluoride can also used for the production of ketones [4–6] and enolates [7,8], important inter-mediates in the pharmaceutical industry, and for the production of ionic liquids [9,10], as well as for a wide variety of other organic reactions [11–15].

Benzoyl fluoride can be prepared from a number starting materials. The conversion of benzoic acid to benzoyl fluoride using a fluorinating agent, such as dialkylaminosulfur trifluoride or other deoxofluorinating agents [16–22] or with XeF_2 [23] proceeds with good yields, but requires a large quantity of fluorinating material. Benzoyl fluoride can also be prepared by the reaction of benzoyl chloride with a fluorine source, such as cobaltocenium fluoride [24]. Recent synthetic efforts have shown, as well, that benzo-bromide [25] or iodobenzene [26] will undergo carbonylation to the corresponding benzoyl bromide and iodide, suggesting that benzoyl fluoride could be produced in a similar manner.

The formation of benzoyl fluoride from benzotrifluoride was first demonstrated by Schwertfeger and Siegemund [27]. These authors hypothesized that the reaction of benzotrifluoride with trifluoroacetic acid should proceed in a manner similar to that for the well known reaction of benzotrichloride with trichloroacetic acid – $C_6H_5CCl_3 + CCl_3COOH \rightarrow C_6H_5COCl + CCl_3COCl + HCl$ [28]. Metals, such as aluminum, antimony, and iron in the presence of fluorinated carboxylic acids were found to produce benzoyl fluoride in good yields at temperatures above 463 K. It was also shown that benzotrifluoride could be converted readily to benzoyl fluoride with 90% yield in 20 h in the presence of TiO_2 or $TiCl_4$ and trifluoroacetic acid at 403 K. The formation of benzoyl fluoride from benzotrifluoride was observed in our own work on the oxidative carbonylation of benzotrifluoride to trifluoromethylben-zoic acid. Benzoyl fluoride was produced as a principle byproduct at low temperatures and under mild conditions [29]. VO_2^+ cations present in the system, together with trifluoroacetic acid and its anhydride were identified to be responsible for the conversion of benzotrifluoride to benzoyl fluoride [29]. Since turnover numbers as high as 110 were achieved, the reaction was established to be catalytic. These observations, together with the earlier work of Schwertfeger and Siegemund, provided the stimuli for the present investigation, the aim of which was to investigate the role of oxo species and metal oxides in the catalyzed synthesis of benzoyl fluoride synthesis from benzotrifluoride.

2. Experimental

Into 50 mL Hastelloy C autoclaves was loaded benzotrifluoride (37.5 mmol), trifluoroacetic acid (37.5 mmol), trifluoroacetic anhydride (3.05 mmol), and Nb_2O_5 (0.516 mmol). The autoclave was sealed and purged with helium before pressurizing to 0.345 MPa with O_2. The autoclave was heated to 398 K in about

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10 min and then quenched with ice water to 308 K. Total autoclave operation time was 1 h. The reaction mixture, which often evolved white fumes once the autoclave was opened, was transferred to a scintillation vial and weighed and a small sample was taken for NMR analysis. Water was added to the reaction mixture to extract any remaining trifluoroacetic acid and any HF formed. The sample was centrifuged and decanted. The organic phase was analyzed by GC using a DB-WAX capillary column and an FID detector, by GC/MS, and by ^{19}F NMR. The aqueous phase was analyzed by ^{19}F NMR. The gas phase was collected and analyzed by GC/MS.

3. Results and discussion

Our initial efforts focused on determining the components of the reaction system necessary for the reaction to proceed. As shown in Table 1, NH_4VO_3, CF_3COOH, $(CF_3COO)_2O$, and O_2 are all necessary components of the reaction system required to promote the conversion of benzotrifluoride to benzoyl fluoride and benzoic acid. A small amount of benzoyl fluoride and benzoic acid could be formed in the absence of O_2, but neither of the products was formed in the presence of O_2 and the absence of one of the other three reaction components.

Several metal oxides were found to catalyze the reaction of benzotrifluoride to benzoyl fluoride at 353 K, with a small amount of benzoic acid being produced as a byproduct. As seen in Table 2, the highest product yields were obtained using Nb_2O_5, and the product yields decreased in the order $Nb_2O_5 > NH_4VO_3 > TiO_2 > Sb_2O_3 > ZrO(NO_3)_2 > Sb_2O_5 > VO > MoO_2 > V_2O_5$. It was also seen that with the exception of TiO_2, product yields were generally higher in the presence of O_2, as was the selectivity to benzoyl fluoride. While not shown, experiments were conducted to establish the necessity of having CF_3COOH and $(CF_3COO)_2O$ as components of the reaction system. As in the case of the experimental results presented in Table 1, it was found that both the acid and its anhydride are essential for the reaction to proceed.

Since the highest yield of benzoyl fluoride was obtained using Nb_2O_5, all further experiments were conducted with this material. The effects of reaction temperature on the conversion of benzotrifluoride and the selectivity to benzoyl fluoride are shown in Fig. 1. Reaction temperatures of 373 K or higher were required to achieve high benzotrifluoride conversion. The selectivity to benzoyl fluoride tended to increase with temperature, suggesting that the rate of benzoyl fluoride production increased more rapidly than the rate of benzoic acid formation, and at higher temperatures, a benzoyl fluoride selectivity of approximately 90% selectivity was observed.

The effects of reaction time are shown in Fig. 2 for a temperature of 398 K. When the autoclave was heated to reaction temperature and quenched immediately, approximately 3.5% conversion was obtained and a selectivity of ~96%. After 5 min at reaction temperature, 89% conversion and 93% selectivity was achieved. The conversion approached 100% after 10 min at reaction temperature. A slight decrease in selectivity was observed with time as a result of benzoyl fluoride reacting to form benzoic acid as described above.

A separate experiment was carried out to identify whether benzoic acid was produced as a secondary product from benzoyl fluoride. Benzoyl fluoride was dissolved in toluene and placed in the autoclave together with trifluoroacetic acid at 398 K for 1 h. The observed products included benzoic acid and trifluoroacetyl fluoride. These results suggest that benzoic acid forms from the sequential reaction of benzotrifluoride to benzoyl fluoride, which then reacts further with trifluoroacetic acid to form benzoic acid. The results presented in Fig. 2 indicate that the former reaction

Table 2
Catalyst scoping with and without oxygen present. Reaction conditions: 37.5 mmol benzotrifluoride (5.48 g), 12.9 mmol CF_3COOH (1.48 g), 3.80 mmol $(CF_3CO)_2O$ (0.80 g), 0.516 mmol catalyst, 0.345 MPa O_2, T = 353 K, t = 1 h.

Catalyst	Product	Yield (mmol)		Selectivity (%)	
		With O_2	Without O_2	With O_2	Without O_2
1 Nb_2O_5	Benzoyl fluoride	2.54	Trace	69	54
	Benzoic acid	1.14	Trace		
2 NH_4VO_3	Benzoyl fluoride	1.06	0.03	77	39
	Benzoic acid	0.32	0.05		
3 TiO_2	Benzoyl fluoride	0.82	0.71	81	86
	Benzoic acid	0.20	0.12		
4 Sb_2O_3	Benzoyl fluoride	0.77	0.16	94	51
	Benzoic acid	0.05	0.16		
5 $ZrO(NO_3)_2$	Benzoyl fluoride	0.58	0.26	90	78
	Benzoic acid	0.06	0.07		
6 Sb_2O_5	Benzoyl fluoride	0.41	0.27	90	89
	Benzoic acid	0.05	0.03		
7 VO	Benzoyl fluoride	0.22	0.00	89	23
	Benzoic acid	0.03	0.01		
8 MoO_2	Benzoyl fluoride	0.13	0.01	90	73
	Benzoic acid	0.01	0.00		
9 V_2O_5	Benzoyl fluoride	0.01	[a]	46	
	Benzoic acid	0.01	[a]		

[a] Reaction not conducted.
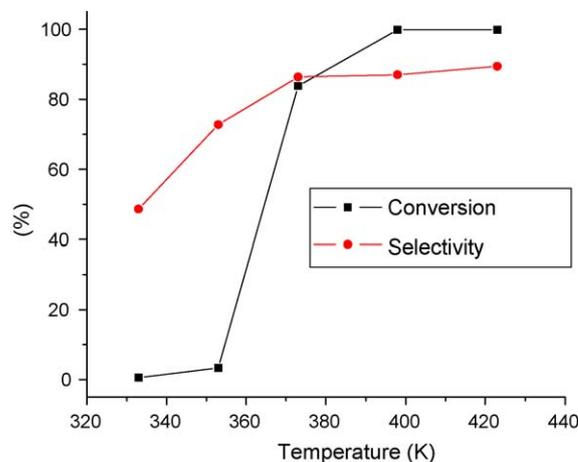
Fig. 1. Nb_2O_5 catalyzed conversion of benzotrifluoride versus temperature. Reaction conditions: 37.6 mmol benzotrifluoride (5.48 g), 37.5 mmol CF_3COOH (4.32 g), 3.80 mmol $(CF_3CO)_2O$ (0.80 g), 0.516 mmol Nb_2O_5 (0.1372 g), 0.345 MPa O_2, t = 1 h.

Table 1
Reactant scoping in the presence of NH_4VO_3 and O_2. Reaction conditions: 37.5 mmol benzotrifluoride (5.48 g), T = 353 K, t = 1 h.

	CF_3COOH (mmol)	$(CF_3CO)_2O$ (mmol)	NH_4VO_3 (mmol)	O_2 (MPa)	Benzoyl fluoride (mmol)	Benzoic acid (mmol)
1	0	0	0.516	0.345	0.00	0.00
2	12.9	0	0.516	0.345	0.00	0.01
3	12.9	3.8	0	0.345	0.01	0.01
4	12.9	3.8	0.516	0	0.03	0.05
5	12.9	3.8	0.516	0.345	1.06	0.32
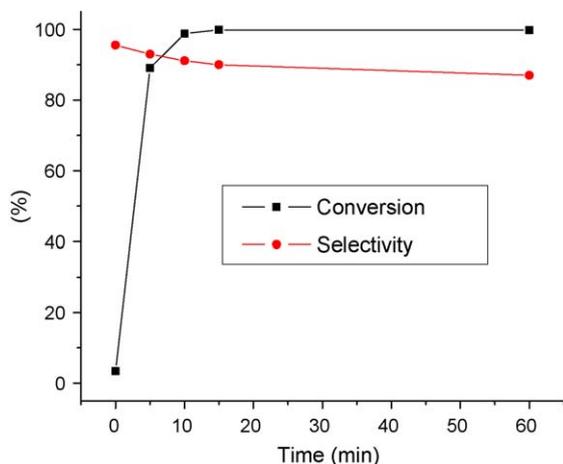
Fig. 2. Conversion of benzotrifluoride versus time. Reaction conditions: 37.6 mmol benzotrifluoride (5.48 g), 37.5 mmol CF$_3$COOH (4.32 g), 3.80 mmol (CF$_3$CO)$_2$O (0.80 g), 0.516 mmol Nb$_2$O$_5$ (0.1372 g), 0.345 MPa O$_2$ T = 398 K.

proceeds at a higher rate than the later, and the results presented in Fig. 1 indicate that the activation energy for the former reaction is higher than for the latter.

Since trifluoroacetic acid and its anhydride were found to be essential components of the reaction system required for the conversion of benzotrifluoride to benzoyl fluoride, the role of acid pKa was investigated. The underlying hypothesis was that the acid is necessary to activate the CF$_3$ group of benzotrifluoride. To test this hypothesis, acids with pKa values ranging from that of acetic acid (pKa = +5) to that methanesulfonic acid (pKa = −2) were examined. The conversion of benzotrifluoride and the selectivity to benzoyl fluoride are presented in Fig. 3a and b, respectively. When acetic acid was used as the acid, only trace quantities of benzoyl fluoride and benzoic acid were observed, and the system exhibited a benzoyl fluoride selectivity of <10%. The conversion increased to roughly ~10% when chloroacetic acid was used, but the benzoyl fluoride selectivity remained low. Remarkable increases in conversion and selectivity were observed with the use of dichloroacetic acid, trichloroacetic acid, chlorodifluoroacetic acid, trifluoroacetic acid, and methanesulfonic acid. The conversion increased slightly from dichloroacetic acid (~50%) to trifluoroa-cetic acid (~70%). The fluorinated acetic acids, namely chlorodi-fluoroacetic acid, trifluoroacetic acid, and pentafluoropropionic acid, tended to gave higher benzoyl fluoride selectivities (~90%). Such acids were also more stable to than the chlorinated carboxylic acids, dichloroacetic acid and trichloroacetic acid, which tended to decompose to form carbon dioxide above 398 K. Pentafluoropro-pionic acid gave a lower benzoyl fluoride conversion (~30%) compared to the trifluoroacetic acid, but exhibited the highest benzoyl fluoride selectivity (~92%). Relatively high benzotriflour-ide (~60%) conversion benzoyl selectivity (~76%) were obtained as well with methanesulfonic acid. Taken together, these results support the hypothesis that the conversion of benzotrifluoride increases with the acid strength. The decrease in activity of the pentafluoropropionic acid, the acidity of which is comparable to that of trifluoroacetic acid may reflect a more complicated role of the acid than simply serving as a proton source to activate the C–F bond of benzotrifluoride.

The effect of acid concentration was also investigated. It was observed that if the concentration of trifluoroacetic acid was less than one equivalent of benzotrifluoride, then the conversion of this reactant was limited by the concentration of acid. However, if the ratio of trifluoroacetic acid to benzotrifluoride exceeded unity, then all of the latter reagent could be consumed. These observations are consistent with the following reaction stoichio-

Fig. 3. (a) Conversion of benzotrifluoride using Nb$_2$O$_5$ in the presence of various acids. Reaction conditions: 37.6 mmol benzotrifluoride (5.48 g), 12.9 mmol acid, 12.9 mmol corresponding anhydride, 0.516 mmol Nb$_2$O$_5$ (0.1372 g), 0.345 MPa O$_2$, T = 353 K, t = 4. (b) Selectivity of benzotrifluoride to benzoyl fluoride using Nb$_2$O$_5$ in the presence of various acids. Reaction conditions: 37.6 mmol benzotrifluoride (5.48 g), 12.9 mmol acid, 12.9 mmol corresponding anhydride, 0.516 mmol Nb$_2$O$_5$ (0.1372 g), 0.345 MPa O$_2$, T = 353 K, t = 4.

metry proposed by Schwertfeger and Siegemund by analogy to the well-known reaction of benzotrichloride to benzoyl chloride [27,28]:
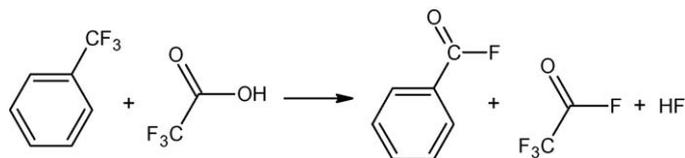
Confirmation of the proposed reaction stoichiometry was obtained from analysis of the liquid phase products by ^{19}F NMR and analysis of the autoclave headspace by GC/MS. ^{19}F NMR confirmed the formation of benzoyl fluoride, observed as a peak at 17.62 ppm, and the consumption of benzotrifluoride, observed as a peak at −63.16 ppm. A very small peak was also observed at 64.24 ppm, attributable to HF. Analysis of the headspace by GC/MS revealed the presence of O$_2$ together with small amounts of carbonyl fluoride, benzoyl fluoride, and a large quantity of trifluoroacetyl fluoride, identified by m/z peaks at 116, 97, 69, 50, 47, 31, and 28 [30,31]. Observation of a significant concentra-tion of trifluoroacetyl fluoride in the head space supports the proposed stoichiometry. At the same time, the absence of a large concentration of HF in the autoclave headspace, is likely due to the

Table 3
Influence of oxygen and Nb_2O_5 loading on conversion and selectivity. Reaction conditions: 37.5 mmol benzotrifluoride (5.48 g), 37.5 mmol CF_3COOH (4.32 g), 3.80 mmol $(CF_3CO)_2O$ (0.80 g), $T = 398$ K, $t = 1$ h.

Entry	Nb_2O_5 (mmol)	O_2 (MPa)	Conversion (%)	Selectivity (%)
1	0.516	0.35	99.8	87
2	0.516	0	98.3	86
3	0.101	0.35	84.0	87
4	0.101	0	27.6	90
5	0.037	0.35	47.3	83
6	0.037	0	13.8	81
7	0.018	0.35	1.2	66
8	0.018	0	0.1	48

reaction of HF with trifluoroacetic anhydride to form trifluoroacetyl fluoride and trifluoroacetic acid [32]. The occurrence of this latter reaction suggests that less than a stoichiometric quantity of trifluoroacetic acid could be loaded into the autoclave, since the additional required acid could be generated from the reaction of HF with the anhydride.

It is notable that the above reaction stoichiometry does not involve O_2, and yet, as reported in Table 2, product yield and benzoyl fluoride selectivity were higher in the presence of O_2. To further explore this issue, the experiments reported in Table 3 were carried out. With high Nb_2O_5 loadings and excess trifluoroacetic acid, a conversion of 99.8% and a selectivity of 87% were obtained in the presence of oxygen (entry 1) and a conversion of 98.3% and a selectivity of 86% were obtained in the absence of oxygen (entry 2). With lower catalyst loadings, a clear dependence on oxygen was observed, with reactions proceeding at a higher rate in the presence of molecular oxygen (entries 3, 5, and 7) than reactions carried out in the absence of molecular oxygen (entries 4, 6, and 8).

To determine the role of oxygen, a reaction was conducted using $^{18}O_2$ under conditions otherwise identical to those of entry 1 in Table 2. In agreement with the results for the identical experiment carried out using $^{16}O_2$, the benzotrifluoride conversion and benzoyl fluoride selectivity were found to be 99.8% and 85%, respectively. The gas phase was collected and analyzed by GC/MS. No labeled ^{18}O was observed in the trifluoroacetyl fluoride, and only $^{18}O_2$ and a small quantity of $^{16}O_2$, due to some residual air retained in the autoclave headspace, but no $^{18}O^{16}O$ were detected. The liquid phase was similarly analyzed by GC/MS, and here too ^{18}O was not observed in the benzoyl fluoride or in the benzoic acid. These results clearly indicate that while molecular oxygen may play a role as a fluorine transfer agent, it is not consumed during the course of the reaction. Since no $^{16}O^{18}O$ was observed, it is inferred that molecular O_2 does not exchange ^{18}O atoms with unlabeled oxygen present in Nb_2O_5.

Taken together, the preceding results suggest that the conversion of benzotrifluoride to benzoyl fluoride proceeds via the reaction of an H atom on trifluoroacetic acid with one of the F atoms on benzotrifluoride to form HF and the exchange of an O atom for an F atom by reaction of the residual trifluoroacetate anion and benzodifluoro cation. This view suggests that trifluoroacetic acid acts as an oxygen transfer agent and the acceptor of an F atom to form trifluoroacetyl fluoride, in addition to serving to activate the CF_3 group of benzotrifluoride.

A possible mechanism for the conversion of benzotrifluoride to benzoyl fluoride is presented in Scheme 1. In the first step, trifluoroacetic acid and benzotrifluoride coordinate to the niobium oxide catalyst. In the second step, a hydrogen bond is formed between the trifluoroacetic acid and the fluorine in the methyl group of the benzotrifluoride. Interaction of these species with the niobium oxide catalyst stabilizes them. In step 3, the C–F bond is broken, and HF is released into solution, where it then reacts with
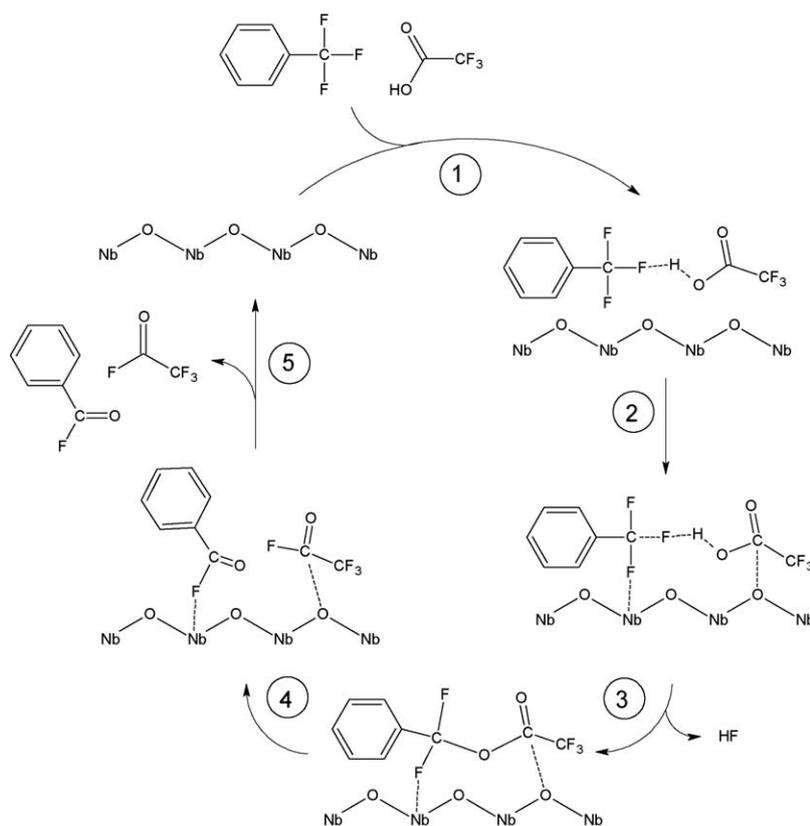
Scheme 1.

trifluoroacetic anhydride. Step 4 involves the formation of a species similar to an ester on the surface of the niobium catalyst. The catalyst assists in fluorine–oxygen transfer (step 5), leading to the formation of benzoyl fluoride and trifluoroacetyl fluoride bound to the surface of the niobium oxide. Molecular oxygen loosely coordinated to the catalyst is envisioned to facilitate the transfer of fluorine during this step, perhaps through the formation of FO_2 as an intermediate [33]. Finally, the benzoyl fluoride and trifluoroacetyl fluoride desorb from the surface of the catalyst. Benzoyl fluoride accumulates in the liquid phase, whereas trifluoroacetyl fluoride accumulates in the gas phase.

The reaction is thought to proceed through a similar mechanism for the other heterogeneous catalysts listed in Table 2. In the case of the NH_4VO_3, which dissolves completely, it is envisioned that coordination of benzotrifluoride and trifluoroacetic acid to VO_2^+ cations facilitates the exchange of O and F atoms in a manner similar to that seen in steps 3 and 4 of Scheme 1. The superior activity of Nb_2O_5 relative to the other oxides investigated is attributed to the presence of strong Lewis acid-base pairs at the surface of the catalyst. Strongly Lewis acidic Nb^{5+} cations would be expected to favor the stabilization of adsorbed benzotrifluoride, whereas strongly Lewis basic O^{2-} anion would favor the stabilization of adsorbed trifluoroacetic acid.

4. Conclusions

The present work has led to a novel, highly active and selective method for converting benzotrifluoride to benzoyl fluoride. The process operates in the presence of molecular oxygen with Nb_2O_5 as the most active catalyst, although other transition metal oxides are also capable of catalyzing the reaction. The halogenated acid serves two roles. The first it to protonate and thereby activate the otherwise quite stable CF_3 group of the benzoyl fluoride, making the C–F bond more susceptible to attack. The acid participates in O–F exchange in the presence of the catalyst to form benzoyl fluoride and the acetyl fluoride of the acid. Oxygen facilitates the fluorine transfer but does not dissociate or enter into the reaction products. Likewise, there is no evidence for oxygen exchange between O_2 and Nb_2O_5. The anhydride consumes the HF formed during the reaction to form the corresponding acid and acetyl fluoride.

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