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Synthesis and Properties of New Perfluorinated Aliphatic Isocyanides

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Although the first fluorinated isocyanide, $CF_3N{\equiv}C$, was first synthesized in 1967,[1] synthesis of other fluorine-containing analogues and, in particular, a study of their chemistry has occurred only in more recent years. This chemistry has been recently reviewed.[2] Known perfluorinated isocyanides include $CF_3N{\equiv}C$, $C_6F_5N{\equiv}C$,[3] $SF_5N{\equiv}C$,[4] and $CF_2{=}CFN{\equiv}C$.[5]

α-Dehalogenation of the corresponding dibromomethanimine (by using Mg in THF) gives rise to $CF_3N{\equiv}C$ in excellent yield but to much lower yields of C_6F_5NC and SF_5NC.[3,4] Vacuum pyrolysis at 240 °C of $CF_2{=}CFNCCr(CO)_5$ leads smoothly to $CF_2{=}CFNC$.[2] All of these isocyanides are very unstable compounds which tend to decompose at relatively low temperatures to form polymeric materials.[2,6]

We find that the defluorination of perfluoroazaalkenes with Ph_3P not only provides a more straightforward route to the previously known $CF_3N{\equiv}C$, but also allows the synthesis of the previously unknown higher homologues $C_2F_5N{\equiv}C$ (**1**) and $C_3F_7N{\equiv}C$ (**2**). The synthesis of the precursors used in our method, $R_fN{=}CF_2$,[7,8] requires fewer steps, and the production of the isocyanides does not require the use of a solvent.[9]

The previously described route to $CF_3N{\equiv}C$ required the conversion of $CF_3N{=}CF_2$ into the dibromomethanimine $CF_3N{=}CBr_2$ via a three step synthesis which was achieved by the utilization of BBr_3.[10]

Results and Discussion

The ease of synthesis of perfluoroazaalkenes[7,8] makes this family of compounds attractive precursors to a large number of interesting materials.

$$ClCN + SF_4 + CsF \xrightarrow[-CsCl]{160\ ^\circ C} CF_3N{=}SF_2$$

$$CF_3N{=}SF_2 + 2ClF \xrightarrow[-SF_4]{} CF_3NCl_2$$

$$CF_3NCl_2 + CF_2{=}CFCl \xrightarrow{70\ ^\circ C} CF_3N(Cl)CF_2CFCl_2$$

$$CF_3N(Cl)CF_2CFCl_2 \xrightarrow[-CFCl_3]{h\nu} CF_3N{=}CF_2$$

For the higher homologues, the perfluoroalkyl nitriles are commercially available. In the synthesis, the alkyl chain length is increased by one CF_2 unit.

$$R_fCN + 2ClF \rightarrow R_fCF_2NCl_2$$

$$R_fCF_2NCl_2 + CF_2{=}CFCl \xrightarrow{70\ ^\circ C} R_fCF_2N(Cl)CF_2CFCl_2$$

$$R_fCF_2N(Cl)CF_2CFCl_2 \xrightarrow[-CFCl_3]{h\nu} R_fCF_2N{=}CF_2$$

$$R_f = CF_3, C_2F_5$$

The high phosphorus-fluorine bond energy renders triphenylphosphane a superb defluorinating reagent. We have used this reagent to provide a simpler route to isocyanides, e.g.

$$CF_3N{=}CF_2 \xrightarrow[-Ph_3PF_2]{-Ph_3P} \underset{80-90\%}{CF_3N{\equiv}C}$$

The IR and ^{19}F NMR spectral data obtained agree with the literature.[10] Similarly the higher homologues are converted to isocyanides **1** and **2**.

$$C_2F_5N{=}CF_2 \xrightarrow[-Ph_3PF_2]{+Ph_3P} \underset{(1)\ 20\%}{C_2F_5N{\equiv}C} + \underset{80\%}{CF_3CF{=}NCF_3}$$

$$C_3F_7N{=}CF_2 \xrightarrow[-Ph_3PF_2]{+Ph_3P} \underset{(2)\ 40\%}{C_3F_7N{\equiv}C} + \underset{60\%}{C_2F_5CF{=}NCF_3}$$

The yields of **1** and **2** are markedly impacted by the isomerization of their precursors which is catalyzed irreversibly by the presence of fluoride ion. These compounds are characterized by comparison with IR and ^{19}F NMR spectral data given in the literature.[11] This isomerization still occurs even when the experimental conditions are changed by using solvents such as acetonitrile or benzonitrile or by carrying out the reaction at lower temperatures.

For the new isocyanides, the IR spectra show absorption bands for the isocyanide stretching frequency at 2120 cm^{-1} for **1** and 2114 cm^{-1} for **2** compared with 2127 cm^{-1} for $CF_3N{\equiv}C$. The ^{19}F resonances for the CF_2 group bonded to $N{\equiv}C$ show the characteristic line-broadening from coupling to ^{14}N which is normally observed for isocyanides. The CF_2 groups in CF_3CF_2NC at −91.0 ppm and in $CF_3CF_2CF_2NC$ at −87.1 ppm, appear as triplets ($^2J_{F-N} = 13$ Hz). The mass spectrum of both compounds shows M^+.

The stabilities of **1** and **2** are similar to that of $CF_3N{\equiv}C$. When stored at temperatures above −78 °C, decomposition occurs to form a nonvolatile oil. At +25 °C either neat or in solution with nonpolar, noncoordinating solvents, oligomerization occurs readily. However, solutions of the isocyanides in polar solvents, such as acetonitrile or benzonitrile, are stable at 25 °C for several hours.

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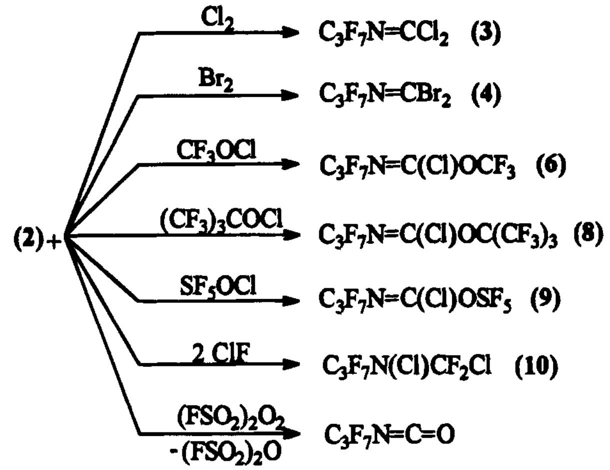
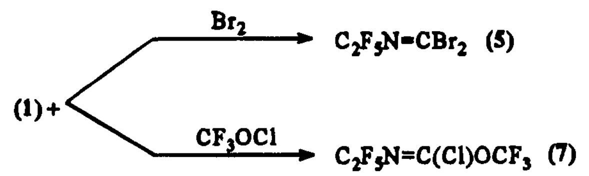
The isocyanides react with oxidizing agents to give the following products as colorless liquids in 90–95% yield.





These reactions are complete after warming the mixture slowly from −196 °C to room temperature. No reaction takes place with iodine or $(CF_3)_2NCl$ because of their lower oxidizing strength. Because ClF is a powerful oxidizer, it was not possible to isolate the 1:1 addition product $C_3F_7N{=}CFCl$. In all other reactions we observe a 1:1 addition. Even with excess reagent, no *N*-chloroamines are formed. Similar behavior is reported for the reaction between perfluorinated nitriles and hypochlorites,[12] although further reaction occurs at elevated temperatures. The new products are characterized by IR, ^{19}F NMR, and mass spectroscopy. The isocyanate C_3F_7NCO was identified by comparison with literature data.[11]

Experimental Section

Materials. The chemicals Ph_3P, Cl_2, Br_2, and I_2 (Aldrich Chemical Co. Inc.); ClCN (Solkatronic Chemicals Inc.); ClF and SF_4 (Atochem North America); CF_3CN, C_2F_5CN, and $CF_2{=}CFCl$, COF_2 (PCR) were purchased and used as received. The compounds $(FSO_2)_2O_2$ and $(CF_3)_2CO$ are gifts from Professor Felix Aubke and Central Glass Ltd. The reagents $(CF_3)_2NCl$, CF_3OCl, $(CF_3)_3COCl$, and SF_5OCl are prepared by the reaction of ClF with $CF_3N{=}CF_2$,[7] COF_2,[13,14] $(CF_3)_3COK$,[15–17] and SOF_4,[13,18] respectively. The perfluoroazaalkenes, $CF_3N{=}CF_2$,[7] $C_2F_5N{=}CF_2$,[7] and $C_3F_7N{=}CF_2$[8] are also prepared by literature methods.

General Procedures. A conventional vacuum system, consisting of a Pyrex glass vacuum line fitted with Teflon needle stopcocks and equipped with Heise Bourdon tube and Televac thermocouple gauges, is used to handle gases and volatile liquids. Standard *PVT* techniques are used to quantitate starting materials or products. Fractional condensation (trap-to-trap distillation) is used for the purification of products. Infrared spectra are recorded on a Perkin-Elmer 1710 FT-IR spectrometer using a 10-cm glass cell equipped with KBr windows. ^{19}F-NMR spectra are obtained on a Bruker AC200 or AC300 FT-NMR instrument using CD_3CN or $CDCl_3$ as solvent. Chemical shifts are reported with respect to $CFCl_3$. Mass spectra are obtained with a Varian VG 7070 HS mass spectrometer by using electron impact or chemical ionization techniques. Peak assignments of the chlorine- and bromine-containing fragments are based on ^{35}Cl and ^{79}Br, respectively. Elemental analyses were performed by Beller Mikroanalytisches Laboratorium, Göttingen, Germany.

Preparation of the Isocyanides $CF_3N{\equiv}C$, $CF_3CF_2N{\equiv}C$ (1) and $CF_3CF_2CF_2N{\equiv}C$ (2). Into 5 mmol of triphenylphosphane, in a round-bottomed flask with a stirrer, is condensed 5 mmol of $R_fN{=}CF_2$. After a slow warmup from −196 to +25 °C, the mixture is stirred at 25 °C for 30 min. A mixture of $R_fN{=}CF_2$ and $CFCl_3$ can also be used. All volatile material is then removed under vacuum from the red-brown residue and distilled through a trap at −115 °C. The isocyanides can be purified further by repeated distillation through a trap at −120 °C to separate them from the byproducts $CF_3CF{=}NCF_3$ (in the case of C_2F_5NC) and $C_2F_5CF{=}NCF_3$ (in the case of C_3F_7NC). Yields range from 80–90% ($R_f = CF_3$), to 40–50% ($R_f = C_3F_7$), and to 20–30% ($R_f = C_2F_5$). Each of these isocyanides is a colorless liquid at low temperature and storage at −78 °C is required. Otherwise oligomerization occurs.

Properties of $CF_3CF_2N{\equiv}C$ (1). Compound **1** is isolated in a trap at −196 °C, after having passed a trap at −120 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 2120 s ($\nu_{N\equiv C}$), 1363 m, 1310 w, 1246 vs, 1196 vs, 1160 m, 1074 vs, 982 w, 930 m, 922 m, 889 w, 692 m. ^{19}F NMR (CD_3CN): δ −86.1 (CF_3, s); −91.0 (CF_2, t), $^2J_{F,N}$ = 13.1 Hz. MS EI [*m/e* (species), intensity]: 145 (M^+), 2; 126 ($M^+ - F$), 7; 119 ($C_2F_5^+$), 15; 100 ($C_2F_4^+$), 3; 76 (CF_2NC^+), 65; 69 (CF_3^+), 100.

Properties of $CF_3CF_2CF_2N{\equiv}C$ (2). Compound **2** is isolated in a trap at −196 °C, after having passed a trap at −120 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 2114 m ($\nu_{N\equiv C}$), 1355 m, 1295 w, 1248 vs, 1215 m, 1175 m, 1129 m, 1084 w, 987 m, 960 m, 847 m, 735 m. ^{19}F NMR (CD_3CN): δ −80.1 (CF_3, t), $^4J_{F,F}$ = 8.5 Hz; −87.1 (CF_2N, t), $^2J_{F,N}$ = ~13 Hz; −127.2 (CF_2, s). MS EI [*m/e* (species), intensity]: 195 (M^+), 1; 169 ($C_3F_7^+$), 20; 131 ($C_3F_5^+$), 12; 119 ($C_2F_5^+$), 51; 100 ($C_2F_4^+$), 18; 76 (CF_2NC^+), 93; 69 (CF_3^+), 100.

General Procedure for Reactions of 1 and 2 with Oxidizers. Equimolar mixtures of R_fNC and reagents are condensed into a glass vessel, warmed slowly to room temperature, and kept for 10–30 min at 25 °C. Distillation through traps at −60 to −80 °C (−110 °C in the case of C_3F_7NCO) gives pure products. Yields of the colorless liquids are approximately 90–95%.

Properties of $CF_3CF_2CF_2N{=}CCl_2$ (3). Compound **3** stops in a trap at −80 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 1681/1662 s ($\nu_{N=C}$), 1354 m, 1320 m, 1289 m, 1240 vs, 1206 s, 1186 s, 1137 s, 1083 w, 990 s, 925 s, 848 m, 779 m, 736 s, 678 w, 645 w, 610 w. ^{19}F NMR ($CDCl_3$): δ −81.0 (CF_3, t), $^4J_{F,F}$ = 8.4 Hz; −97.9 (CF_2N, qt); −129.1 (CF_2, t), $^3J_{F,F}$ = 2.8 Hz. MS CI [*m/e* (species), intensity]: 266 (MH^+), 59; 246 ($M^+ - F$), 81; 230 ($M^+ - Cl$), 80; 196 ($C_3F_7NCH^+$), 14; 185 ($C_3F_6Cl^+$), 25; 169 ($C_3F_7^+$), 52; 146 ($M^+ - C_2F_5$), 78; 119 ($C_2F_5^+$), 13; 100 ($C_2F_4^+$), 16; 85 (CF_2Cl^+), 37; 76 (CF_2NC^+), 36; 69 (CF_3^+), 100.

Properties of $CF_3CF_2CF_2N{=}CBr_2$ (4). Compound **4** stops in a trap at −60 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 1711/1645 s ($\nu_{N=C}$), 1353 s, 1322 w, 1287 w, 1242 vs, 1204 m, 1178 m, 1135 s, 1029 w, 987 s, 856 m, 834 m, 766 w, 717 m. ^{19}F NMR ($CDCl_3$): δ −80.9 (CF_3, tt), $^4J_{F,F}$ = 8.7 Hz, $^3J_{F,F}$ = 1.4 Hz; −99.0 (CF_2N, qt); −128.9 (CF_2, tq), $^3J_{F,F}$ = 3.1 Hz. MS CI [*m/e* (species), intensity]: 354 (MH^+), 11; 334 ($M^+ - F$), 14; 274 ($M^+ - Br$), 85; 229 ($C_3F_6Br^+$), 13; 196 ($C_3F_7NCH^+$), 30; 169 ($C_3F_7^+$), 79; 119 ($C_2F_5^+$), 17; 100 ($C_2F_4^+$), 11; 76 (CF_2NC^+), 32; 69 (CF_3^+), 100. Anal. Calcd for $C_4Br_2F_7N$: C, 13.54; F, 37.48. Found: C, 13.65; F, 37.2.

Properties of $CF_3CF_2N{=}CBr_2$ (5). Compound **5** stops in a trap at −60 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 1715/1652/1642 s ($\nu_{N=C}$), 1384 w, 1351 m, 1236 vs, 1192 s, 1181 s, 1168 s, 1132 m, 1084 s, 1029 s, 988 w, 852 s, 784 w, 737 m, 703 m, 664 w, 627 w. ^{19}F NMR ($CDCl_3$): δ −85.9 (CF_3, t), $^3J_{F,F}$ = 1.1 Hz; −102.8 (CF_2, q). MS CI [*m/e* (species), intensity]: 304 (MH^+), 9; 284 ($M^+ - F$), 15; 224 ($M^+ - Br$), 88; 146 ($C_2F_5NCH^+$), 56; 119 ($C_2F_5^+$), 94; 100 ($C_2F_4^+$), 6; 79 (Br^+), 13; 76 (CF_2NC^+), 38; 69 (CF_3^+), 100.

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Properties of $CF_3CF_2CF_2N{=}C(Cl)OCF_3$ (6). Compound **6** stops in a trap at −70 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 1726/1708 s ($\nu_{N=C}$), 1355 m, 1332 w, 1293 s, 1247 vs, 1206 s, 1138 vs, 1031 w, 995 s, 893 m, 873 w, 857 m, 819 w, 756 m, 739 m, 676 m, 647 w, 535 w. ^{19}F NMR ($CDCl_3$): δ −59.1 (CF_3O, s); −81.1 (CF_3, t), $^4J_{F,F} = 7.9$ Hz; −97.5 (CF_2N, mult.); −129.8 (CF_2, t), $^3J_{F,F} = 4.1$ Hz. MS CI [*m/e* (species), intensity]: 316 (MH^+), 14; 296 ($M^+ - F$), 33; 280 ($M^+ - Cl$), 10; 246 ($M^+ - CF_3$), 2; 230 ($M^+ - OCF_3$), 4; 212 ($C_3F_7NCOH^+$), 7; 196 ($C_3F_7NCH^+$), 26; 192 ($C_3F_6NCO^+$), 17; 169 ($C_3F_7^+$), 15; 119 ($C_2F_5^+$), 11; 100 ($C_2F_4^+$), 7; 86 (CF_3OH^+), 100; 76 (CF_2NC^+), 7; 69 (CF_3^+), 89.

Properties of $CF_3CF_2N{=}C(Cl)OCF_3$ (7). Compound **7** stops in a trap at −80 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 1727/1709 s ($\nu_{N=C}$), 1390 w, 1356 m, 1295 s, 1258 vs, 1237 vs, 1199 s, 1172 s, 1147 vs, 1079 s, 901 m, 878 w, 766 w, 736 m, 677 m, 585 w. ^{19}F NMR ($CDCl_3$): δ −59.2 (CF_3O, s); −86.9 (CF_3, s); −101.1 (CF_2, s). MS CI [*m/e* (species), intensity]: 266 (MH^+), 2; 246 ($MH^+ - F$), 7; 196 ($M^+ - CF_3$), 3; 180 ($M^+ - OCF_3$), 4; 162 ($C_2F_5NCOH^+$), 2; 146 ($C_2F_5NCH^+$), 4; 119 ($C_2F_5^+$), 10; 86 (CF_3OH^+), 100; 69 (CF_3^+), 22.

Properties of $CF_3CF_2CF_2N{=}C(Cl)OC(CF_3)_3$ (8). Compound **8** stops in a trap at −60 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 1730 s/1715 s/1698 m ($\nu_{N=C}$), 1379 m, 1353 m, 1282 vs, 1247 vs, 1208 s, 1159 s, 1138 s, 1122 s, 1072 w, 1009 m, 981 s, 842 s, 754 m, 733 m, 539 w. ^{19}F NMR ($CDCl_3$): δ −68.6 ($(CF_3)_3C$, s); −81.0 (CF_3, t), $^4J_{F,F} = 9.0$ Hz; −97.1 (CF_2N, q); −128.9 (CF_2, s). MS CI [*m/e* (species), intensity]: 466 (MH^+), 16; 446 ($M^+ - F$), 75; 430 ($M^+ - Cl$), 28; 346 ($M^+ - C_2F_5$), 38; 258 ($M^+ - 3CF_3$), 5; 230 ($M^+ - (CF_3)_3CO$), 7; 169 ($C_3F_7^+$), 23; 131 ($C_3F_5^+$) 15; 119 ($C_2F_5^+$), 6; 100 ($C_2F_4^+$), 8; 85 (CF_3O^+), 12; 69 (CF_3^+), 100.

Properties of $CF_3CF_2CF_2N{=}C(Cl)OSF_5$ (9). Compound **9** stops in a trap at −70 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 1723/1698 s ($\nu_{N=C}$), 1354 m, 1329 w, 1246 vs, 1203 s, 1158 s, 1136 s, 1114 s, 992 m, 940 vs, 865 s, 757 m, 738 m, 600 s. ^{19}F NMR ($CDCl_3$): δ 69.5 (SF_4, c), $^2J_{F,F} = 156.5$ Hz; 60.2 (SF, c); −81.0 (CF_3, t), $^4J_{F,F} = 8.0$ Hz; −97.7 (CF_2N, br); −129.6 (CF_2, t), $^3J_{F,F} = 4.0$ Hz. MS CI [*m/e* (species), intensity]: 354 ($M^+ - F$), 3; 254 ($M^+ - C_2F_5$), 6; 230 ($M^+ - OSF_5$), 34; 212 ($C_3F_6NCClH^+$), 36; 192 ($C_3F_6NCO^+$), 73; 169 ($C_3F_7^+$), 17; 142 ($C_2F_4NCO^+$), 8; 127 (SF_5^+), 100; 119 ($C_2F_5^+$), 6; 105 (SOF_3^+), 7; 100 ($C_2F_4^+$), 3; 92 (CF_2NCO^+), 94; 89 (SF_3^+), 80; 69 (CF_3^+), 29. Anal. Calcd for $C_4F_{12}ClNOS$: C, 12.86; F, 61.03. Found: C, 13.33; F, 59.5.

Properties of $CF_3CF_2CF_2N(Cl)CF_2Cl$ (10). Compound **(10)** stops in a trap at −80 °C. Spectral data are as follows. IR (gas) (cm^{-1}): 1352 m, 1306 m, 1255 vs, 1205 s, 1161 s, 1139 s, 1053 s, 1038 s, 993 m, 888 w, 845 w, 809 m, 740 m. ^{19}F NMR ($CDCl_3$): δ −35.0 (CF_2Cl, tt), $^2J_{F,F} = 21.5$ Hz, $^4J_{F,F} = 5.5$ Hz; −81.3 (CF_3, t), $^4J_{F,F} = 9.0$ Hz; −97.5 (CF_2N, mult); −129.0 (CF_2, t), $^3J_{F,F} = 4.2$ Hz. MS CI [*m/e* (species), intensity]: 266 ($C_3F_7NClCHCl^+$), 13; 246 ($C_3F_6NClCCl^+$), 25; 230 ($C_3F_7NCCl^+$), 26; 196 ($C_2F_4NClCCl^+$), 7; 185 ($C_3F_6Cl^+$), 10; 169 ($C_3F_7^+$), 24; 146 ($CF_2NClCCl^+$), 33; 119 ($C_2F_5^+$), 15; 85 (CF_2Cl^+), 22; 69 (CF_3^+), 100.

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