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1,2-Dibromotetrafluoroethane BrCF₂CF₂Br

Purity	97%
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CAS Number 124-73-2

Molecular Formula C2Br2F4

Molecular Weight 259.82

Synthesizing tetrafluoroethylene (abb: TFE) by debrominating 1,2-dibromotetrafluoroethane has the advantage of being O2-free, and is often employed as a laboratory synthesis method.

$$BrCF_2CF_2Br + Zn \xrightarrow{a} CF_2=CF_2 + ZnBr_2$$

In addition, while investigating the synthesis of functional fluoroalkyl compounds from the carbanion of TFE using a nucleophile, it is discovered that CO2 is a useful scavenger for improving selectivity as long as it has an equilibrium relationship with the nucleophile. It is assumed that CN- forms a reversible complex with CO2, resulting in industrially useful cyanotetrafluoropropionic acid ester.

$$NCCOO^- \stackrel{b}{\Longrightarrow} NC^- + CO_2$$

$$NC^- + CF_2 = CF_2 \xrightarrow{c} NCCF_2CF_2$$

 $NCCF_2CF_2^- + CO_2 \xrightarrow{c} NCCF_2CF_2COO^-$

 $NCCF_2CF_2COO^- + (CH_3O)_2SO_2 \xrightarrow{d} NCCF_2CF_2COOCH_3$

- a. DMA 1.6L + Zn 25g + Cu(OAc)2 10g + H2SO4 * 120-60°C 1hr keep + BrCF2CF2Br 1200g dropwise
- b. DMSO, 50°C*2hr,
- c. NaCN 0.50 mol + DMSO + CO2 0.52 mol + CF2=CF2 0.50 mol, -25° C $^{\sim}$ 30°C*1hr + 50°C*1hr
- d. (CH3O)2SO2 0.55 mol * RT

b.~d. overall yield; 72%

Synthesis of fluoro-organic compounds Vol.1, 2010, p106, Moscow (in Russian, by P&M-Invest LLC), Progress in Polym. Sc., 29, 2, 2004, p75-106, J. Am. Che, Soc., 1984, 106, 5544-5546, J. Org. Chem. 1986, 51, p326-332

Properties:

Application

Appearance Liquid **Boiling point, °C** 46-48

Packing:

UN, PG: