Green Chemistry, also known as sustainable chemistry, is an umbrella concept that describes the search for reducing or even eliminating the use of substances in chemical products and reactions which are hazardous to human health and environment. The goal of Green Chemistry is to create a cleaner and more sustainable chemistry, a topic that has received more and more attention in recent years.

Green chemistry searches for alternative, environmentally friendly reaction media (as compared to the traditional organic solvents) and at the same time aims at increased reaction rates, lower reaction temperatures as well higher selectivities (so an overall cost reduction). To the most promising reaction media in this field belong ionic liquids, supercritical CO$_2$ and the use of aqueous media in biphasic systems. In the latter case, the use of phase transfer catalysts or water soluble reactants allows chemists to carry out more and more reactions in aqueous systems. Perfluorinated fluorous solvents/reagents are also found under the Green Chemistry umbrella. Many perfluorinated solvents are neither toxic nor recognized as ozone-depleters, and successfully substitute critical polyhalogenated compounds in many industrial processes. Additionally, highly fluorinated compounds can be used in reactions under supercritical CO$_2$.

Within our Sigma-Aldrich Company, Fluka and Aldrich are proud to offer you a comprehensive collection of products, which can contribute to the search for a greener chemistry, comprising of:

- ionic liquids
- catalysts, ligands, solvents and perfluoro-tags to be used in Fluorous Phase Organic Synthesis (FPOS)
- ammonium- and phosphonium-based reagents, crown ethers and PEG-based reagents, as well as polymer-supported reagents to be used in Phase Transfer Catalysis (PTC)

Each of these topics will be shortly presented, followed by a list of our products.

New offerings are shown and added monthly! When you cannot find the product you are looking for, or for additional technical information, please contact your local Sigma-Aldrich Office (see back cover) or visit our web-site at www.sigma-aldrich.com/fluka

The electronic version of the whole series of ChemFiles can be found under www.sigma-aldrich/chemfiles
Please take a look!

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What are ionic liquids?

- Ionic liquids are organic salts with melting points under 100 °C, often even below room temperature. Recently they are employed more and more as substitute for the traditional organic solvents in chemical reactions. The most common ones are imidazolium and pyridinium derivatives, but phosphonium or tetralkylammonium compounds can also be used for this purpose.

What are their properties?

- Very good dissolution properties for most organic and inorganic compounds
- High thermal stability
- No measurable vapor pressure
- Non-flammable

What are their applications?

- As solvents for synthetic and catalytic purposes, for example Diels-Alder cycloaddition reactions, Friedel-Craft acylation and alkylation, hydrogenation and oxidation reactions and Heck reactions.
- As biphasic systems in combination with an organic solvent or water in extraction and separation technologies.
- For catalyst immobilization without need of special functionalization for the easy recycling of homogeneous catalysts
- As electrolytes in electrochemistry

What are their advantages?

- Optimization of compound characteristics through a broad choice of anion and cation combination (tailor-made solvents)
- Reaction rate enhancement, higher selectivities as well as higher yields
- Used as replacement for Volatile Organic Compounds (VOC) in chemical processes or extractions procedures.

## Product List Ionic Liquids

### Imidazolium derivatives

**R = Methyl**

<table>
<thead>
<tr>
<th>X</th>
<th>CAS No</th>
<th>Name</th>
<th>Formula</th>
<th>Purity, AT, NMR</th>
<th>MP, d^21</th>
<th>M, g</th>
<th>V, mL</th>
</tr>
</thead>
<tbody>
<tr>
<td>MeSO₄</td>
<td>93607</td>
<td>1,3-Dimethylimidazolium methyl sulfate</td>
<td>C₇H₁₅N₂O₂S</td>
<td>≥97.0% (NMR)</td>
<td>52-57°C</td>
<td>208.24 g</td>
<td>5 g; 50 g</td>
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</table>

**R = Ethyl**

<table>
<thead>
<tr>
<th>X</th>
<th>CAS No</th>
<th>Name</th>
<th>Formula</th>
<th>Purity, AT, NMR</th>
<th>MP, d^21</th>
<th>M, g</th>
<th>V, mL</th>
</tr>
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<tbody>
<tr>
<td>Br</td>
<td>89483</td>
<td>1-Ethyl-3-methylimidazolium bromide</td>
<td>C₇H₁₅BrN₂</td>
<td>≥97.0% (AT)</td>
<td>52-57°C</td>
<td>191.07 g</td>
<td>5 g; 50 g</td>
</tr>
<tr>
<td>Cl</td>
<td>272841</td>
<td>1-Ethyl-3-methylimidazolium chloride</td>
<td>C₇H₁₅ClN₂</td>
<td>98%</td>
<td>77-79°C</td>
<td>146.62 g</td>
<td>5 g; 50 g</td>
</tr>
<tr>
<td>PF₆</td>
<td>46093</td>
<td>1-Ethyl-3-methylimidazolium hexafluorophosphate</td>
<td>C₇H₁₅F₆N₄P</td>
<td>≥97.0% (CE)</td>
<td>58-62°C</td>
<td>256.13 g</td>
<td>1 g; 5 g; 50 g</td>
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<tr>
<td>NO₃</td>
<td>04363</td>
<td>1-Ethyl-3-methylimidazolium nitrate</td>
<td>C₇H₁₅N₃O₃</td>
<td>≥99.0% (NT)</td>
<td>38-41°C</td>
<td>173.17 g</td>
<td>1 ml; 5 ml; 50 ml</td>
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<tr>
<td>BF₄</td>
<td>04365</td>
<td>1-Ethyl-3-methylimidazolium tetrafluoroborate</td>
<td>C₇H₁₅BF₄N₂</td>
<td>≥97.0% (T)</td>
<td></td>
<td>197.98 g</td>
<td>d^21: 1.28</td>
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<tr>
<td>CF₃SO₃</td>
<td>04367</td>
<td>1-Ethyl-3-methylimidazolium trifluoromethanesulfonate</td>
<td>C₇H₁₅CF₂N₂O₃S</td>
<td>≥98.0% (T)</td>
<td></td>
<td>260.24 g</td>
<td>d^21: 1.39</td>
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**R = Butyl**

<table>
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<tr>
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<th>CAS No</th>
<th>Name</th>
<th>Formula</th>
<th>Purity, AT, NMR</th>
<th>MP, d^21</th>
<th>M, g</th>
<th>V, mL</th>
</tr>
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<tbody>
<tr>
<td>Br</td>
<td>95137</td>
<td>1-Butyl-3-methylimidazolium bromide</td>
<td>C₈H₁₇BrN₂</td>
<td>≥97.0% (T)</td>
<td>ca 70°C</td>
<td>219.12 g</td>
<td>5 g; 50 g</td>
</tr>
<tr>
<td>Cl</td>
<td>94128</td>
<td>1-Butyl-3-methylimidazolium chloride</td>
<td>C₈H₁₇ClN₂</td>
<td>≥97% (NMR)</td>
<td>ca 55°C</td>
<td>174.67 g</td>
<td>5 g; 50 g</td>
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<tr>
<td>MeSO₄</td>
<td>83086</td>
<td>1-Butyl-3-methylimidazolium methyl sulfate</td>
<td>C₈H₁₇N₂O₂S</td>
<td>≥97.0% (NMR)</td>
<td></td>
<td>250.32 g</td>
<td>d^21: 1.21</td>
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<tr>
<td>PF₆</td>
<td>70956</td>
<td>1-Butyl-3-methylimidazolium hexafluorophosphate</td>
<td>C₈H₁₇F₆N₄P</td>
<td>≥97.0% (NMR)</td>
<td></td>
<td>284.18 g</td>
<td>d^21: 1.37</td>
</tr>
<tr>
<td>BF₄</td>
<td>91508</td>
<td>1-Butyl-3-methylimidazolium tetrafluoroborate</td>
<td>C₈H₁₇BF₄N₂</td>
<td>≥97.0% (NMR)</td>
<td></td>
<td>226.03 g</td>
<td>d^21: 1.22</td>
</tr>
</tbody>
</table>

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R = Hexyl

X = Cl  87929  1-Hexyl-3-methylimidazolium chloride
purum, ≥97.0% (AT) \( \text{C}_9\text{H}_{15}\text{ClN}_3 \) [171058-17-6] M 202.73 \( d^\text{25} : 1.04 \) 5 g; 50 g

X = PF\(_6\)  89320  1-Hexyl-3-methylimidazolium hexafluorophosphate
purum, ≥97.0% (NMR) \( \text{C}_9\text{H}_{15}\text{F}_6\text{N}_3\text{P} \) [304680-35-1] M 312.24 \( d^\text{25} : 1.30 \) 5 g; 50 g

X = BF\(_4\)  73244  1-Hexyl-3-methylimidazolium tetrafluoroborate
purum, ≥97.0% (NMR) \( \text{C}_9\text{H}_{15}\text{BF}_4\text{N}_3 \) [244193-50-8] M 254.08 \( d^\text{25} : 1.15 \) 5 g; 50 g

R = Octyl

X = Cl  95803  1-Methyl-3-octylimidazolium chloride
purum, ≥97.0% (NMR) \( \text{C}_9\text{H}_{15}\text{ClN}_3 \) [64697-40-1] M 230.78 \( d^\text{25} : 1.05 \) 5 g; 50 g

X = BF\(_4\)  96324  1-Methyl-3-octylimidazolium tetrafluoroborate
purum, ≥97.0% (NMR) \( \text{C}_9\text{H}_{15}\text{BF}_4\text{N}_3 \) [244193-52-0] M 282.13 \( d^\text{25} : 1.12 \) 5 g; 50 g

Pyridinium derivatives

\[
\begin{align*}
\text{CH}_3 & \\
\text{N} & \\
R & \\
\text{X}^- & \\
\text{R: Butyl} & \\
\text{X: Cl}^- , \text{BF}_4^- , \text{PF}_6^- \\
\end{align*}
\]

X = Cl  88482  1-Butyl-4-methylpyridinium chloride
purum, ≥97.0% (NMR) \( \text{C}_9\text{H}_{15}\text{ClN} \) [112400-86-9] M 185.7 m.p: 158-160 °C 5 g; 50 g

X = PF\(_6\)  88458  1-Butyl-4-methylpyridinium hexafluorophosphate
purum, ≥97.0% (NMR) \( \text{C}_9\text{H}_{15}\text{F}_6\text{N} \) M 295.21 m.p: ca. 45°C 5 g; 50 g

X = BF\(_4\)  73261  1-Butyl-4-methylpyridinium tetrafluoroborate
purum, ≥97.0% (NMR) \( \text{C}_9\text{H}_{15}\text{BF}_4\text{N} \) [343952-33-0] M 237.05 \( D^\text{25} : 1.2 \) 5 g; 50 g

*Fluka is proud to present a broad selection of ionic liquids. Our range in this rapidly evolving field is continuously expanding. For an overview visit our web site at www.sigma-aldrich.com/fluka*
"Fluorous Phase Organic Synthesis" (FPOS) is a novel separation and purification technique that is attracting great current interest in organic synthesis and process development, e.g. in the immobilization of expensive metal catalysts. The unique physical properties of perfluorinated organic compounds, i.e. their immiscibility that makes them immiscible with water and with many common organic solvents, their ability to form a homogenous solution at elevated temperatures with several of these solvents, their inertness, their solubility in supercritical CO₂ and their ability to dissolve gases contributes to the increasing popularity of the “Fluorous Phase” in organic syntheses.

Catalysis performed in a two-phase reaction mixture consisting of a perfluorinated solvent and an organic solvent, also called “Fluorous Biphase System” (FBS) was first reported by Horváth and Rábai. By introducing perfluorinated ligands a catalyst is solubilized and simultaneously immobilized in the “Fluorous Phase”. By elevating the temperature the biphase system forms a homogenous solution and the catalytic process can take place. Cooling down the reaction mixture leads to the reformation of two separate phases. Afterwards, easy product isolation and the recovery of the perfluoro-tagged metal catalyst can be achieved by simple phase separation (Fig. 1). The isolation and recovery of perfluorinated components can be accomplished not only by a phase separation of immiscible liquid layers but also by solid-liquid extraction using a perfluorinated non-polar stationary phase like “Fluorous Reversed Phase” (FRP) Silica Gel (Fig. 2).

Non-polar perfluorocarbon species show increased solubility in supercritical CO₂ and have been used in the design of CO₂-philic surfactants, chelating agents and ligands in order to improve the solubility of polymers, metals and catalysts. The high solubility of gases, especially oxygen, in perfluorocarbon solvents allows for efficient and selective aerobic oxidation reactions under mild conditions.

The “Fluorous Phase” is also discussed as a promising substitute for the solid phase in combinatorial chemistry. It permits the immobilization of a wide variety of reagents by introducing perfluorinated tags and it enables an easy, efficient isolation and recovery of perfluorinated species by liquid-liquid or solid-liquid extractions.

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**Figure 1:** The Principle of "Fluorous Biphase Catalysis"

**Figure 2:** The Principle of Solid-Liquid-Extration using FRP-Silica

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**References:**

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Catalysts and Ligands

93521  Bis[tris(3-(1H,1H,2H,2H-perfluorodecyl)phenyl)phosphine]palladium(II) dichloride
NEW  ≥90% (AAS)  C_{32}H_{36}Cl_{12}P, Pd  M,3378.55  100 mg; 500 mg

95447  Bis[tris(4-(1H,1H,2H,2H-perfluorodecyl)phenyl)phosphine]palladium(II) dichloride
NEW  ≥80% (AAS)  C_{32}H_{36}C_{12}F_{20}P, Pd  M,3378.55  100 mg; 500 mg

83934  Tris[3-(1H,1H,2H,2H-perfluorodecyl)phenyl]phosphine
NEW  ≥ 95% (GC)  C_{24}H_{24}F_{18}P  M,1600.6  1 g; 5 g

84928  Tris[4-(1H,1H,2H,2H-perfluorodecyl)phenyl]phosphine
NEW  ≥97.0% (GC)  C_{24}H_{24}F_{18}P  M,1600.6  [325459-92-5]  1 g; 5 g

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## Functionalized Perfluoroalkyls ("Fluoro-Tags")

<table>
<thead>
<tr>
<th>Code</th>
<th>Name</th>
<th>CAS Number</th>
<th>Purity</th>
<th>Molecular Formula</th>
<th>Molecular Weight</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>03393</td>
<td>Triacontafluoro-8,10-heptadecanedione</td>
<td>36554-97-9</td>
<td>≥99.0% (NMR)</td>
<td>C₃₀H₁₈F₅₂O₂</td>
<td>808.15</td>
<td>100 mg; 500 mg</td>
</tr>
<tr>
<td>77309</td>
<td>1H,1H,2H,2H-Perfluoroctyl iodide purum, ≥97.0% (GC)</td>
<td>2043-57-4</td>
<td>M₄₇₄</td>
<td>C₁₈H₂₃F₁₁I</td>
<td></td>
<td>5 ml; 25 ml</td>
</tr>
<tr>
<td>87912</td>
<td>1-Bromo-3-(1H,1H,2H,2H-perfluorodecyl)benzene puriss., ≥99.0% (GC)</td>
<td></td>
<td>M₆₀₃.₁₁</td>
<td>C₁₈H₁₃BrF₁₀</td>
<td></td>
<td>1 g; 5 g</td>
</tr>
<tr>
<td>93037</td>
<td>1-Bromo-4-(1H,1H,2H,2H-perfluorodecyl)benzene purum, ≥97.0% (GC)</td>
<td></td>
<td>M₆₀₃.₁₁</td>
<td>C₁₈H₁₃BrF₁₀</td>
<td></td>
<td>1 g; 5 g</td>
</tr>
<tr>
<td>77274</td>
<td>Tridecafluoro-1-iodohexane purum, ≥98% (GC)</td>
<td>355-43-1</td>
<td>M₄₄₅.₉₅</td>
<td>C₉F₁₂I</td>
<td></td>
<td>10 ml; 50 ml</td>
</tr>
<tr>
<td>44,688-2</td>
<td>Perfluorohexyl bromide 98%</td>
<td>335-56-8</td>
<td>M₃₉₈.₉₆</td>
<td>C₉F₁₂Br</td>
<td></td>
<td>1 g; 10 g</td>
</tr>
<tr>
<td>44,686-2</td>
<td>Perfluoroheptyl bromide 98%</td>
<td>365-88-2</td>
<td>M₄₄₈.₉₆</td>
<td>C₁₀F₁₃Br</td>
<td></td>
<td>5 ml; 25 ml</td>
</tr>
<tr>
<td>34,386-2</td>
<td>Perfluoroctylbromide 99.0%</td>
<td>423-55-2</td>
<td>M₄₉₈.₉₇</td>
<td>C₁₁F₁₄Br</td>
<td></td>
<td>1 g; 5 g</td>
</tr>
<tr>
<td>25,784-2</td>
<td>Perfluorodecyliodide 97.0%</td>
<td>423-62-1</td>
<td>M₆₄₅.₉₈</td>
<td>C₁₂F₁₅I</td>
<td></td>
<td>1 g; 5 g</td>
</tr>
<tr>
<td>77289</td>
<td>Heptadecafluoro-1-iodooctane purum, ≥98.0% (GC)</td>
<td>507-63-1</td>
<td>M₅₄₅.₉₆</td>
<td>C₁₀F₁₂I</td>
<td></td>
<td>5 ml; 10 ml; 50 ml</td>
</tr>
<tr>
<td>77269</td>
<td>Pentacosfluoro-1-iodododecane purum, ≥97.0% (GC)</td>
<td>307-60-8</td>
<td>M₇₄₆</td>
<td>C₁₃F₁₅I</td>
<td></td>
<td>1 g; 5 g</td>
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<tr>
<td>42,150-2</td>
<td>Zonyl® PFBE fluorotelomer intermediate 97.0% DuPont product</td>
<td>19430-93-4</td>
<td>M₂₄₆.₀₈</td>
<td>C₈H₁₅F₃</td>
<td></td>
<td>5 g; 25 g</td>
</tr>
<tr>
<td>77307</td>
<td>1H,1H,2H-Perfluoro-1-octene purum, ≥98.0% (GC)</td>
<td>25291-17-2</td>
<td>M₃₄₆.₀₉</td>
<td>C₁₈H₂₃F₁₁</td>
<td></td>
<td>5 ml; 25 ml</td>
</tr>
<tr>
<td>09666</td>
<td>1H,1H,2H-Perfluoro-1-decane purum, ~97% (GC)</td>
<td>21652-58-4</td>
<td>M₄₄₆.₁₁</td>
<td>C₂₀H₂₅F₁₃</td>
<td></td>
<td>25 ml</td>
</tr>
</tbody>
</table>

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### Functionalized Perfluoroalkyls (“Fluoro-Tags”) continued

<table>
<thead>
<tr>
<th>Reference</th>
<th>Name</th>
<th>Formula</th>
<th>CAS Number</th>
<th>Volume(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>77278</td>
<td>1H,1H,2H,2H-Perfluoro-1-octanol purum, ≥97.0% (GC)</td>
<td>C₁₈H₁₈F₁₄O</td>
<td>364.11</td>
<td>5 ml; 25 ml</td>
</tr>
<tr>
<td>77263</td>
<td>1H,1H,2H,2H-Perfluoro-1-decanol pract., ~95% (GC)</td>
<td>C₁₈H₁₈F₁₄O</td>
<td>464.12</td>
<td>1 g; 5 g; 25 g</td>
</tr>
<tr>
<td>77285</td>
<td>Nonfluorovaleric acid pract., ~97% (GC)</td>
<td>C₇H₁₄F₇O₂</td>
<td>264.05</td>
<td>5 ml; 25 ml</td>
</tr>
<tr>
<td>29226</td>
<td>Perfluorocaproic acid purum, ≥97.0% (T)</td>
<td>C₁₀H₁₈F₁₀O</td>
<td>314.06</td>
<td>5 ml; 25 ml</td>
</tr>
<tr>
<td>77260</td>
<td>Pentadecafluorooctanoic acid pract., ~95% (T)</td>
<td>C₁₃H₁₄F₁₂O₂</td>
<td>414.07</td>
<td>10 g; 50 g</td>
</tr>
<tr>
<td>77284</td>
<td>Heptadecafluorononanoic acid</td>
<td>C₁₃H₁₄F₁₂O₂</td>
<td>464.08</td>
<td>5 g; 25 g</td>
</tr>
<tr>
<td>77266</td>
<td>Nonadecafluorodecanoic acid purum, ≥97.0% (T)</td>
<td>C₁₅H₁₄F₁₅O₂</td>
<td>514.08</td>
<td>10 g</td>
</tr>
<tr>
<td>44,677-7</td>
<td>Perfluoroundecanoic acid 95.0%</td>
<td>C₁₅H₁₄F₁₅O₂</td>
<td>564.10</td>
<td>5 g; 25 g</td>
</tr>
<tr>
<td>77267</td>
<td>Perfluorododecanoic acid purum, ≥98.0% (GC)</td>
<td>C₁₆H₁₆F₁₆O₂</td>
<td>614.10</td>
<td>1 g; 10 g</td>
</tr>
<tr>
<td>44,678-5</td>
<td>Perfluorotetradecanoic acid 97.0%</td>
<td>C₁₆H₁₆F₁₆O₂</td>
<td>714.12</td>
<td>5 g; 25 g</td>
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<tr>
<td>40925</td>
<td>Dimethyl(3,3,4,4,5,5,6,6-nonafluoroethyl)chlorosilane DMNFHSCI</td>
<td>C₈H₈ClF₈Si</td>
<td>340.69</td>
<td>2 ml</td>
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### Solvents

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<th>Formula</th>
<th>CAS Number</th>
<th>Volume(s)</th>
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</thead>
<tbody>
<tr>
<td>94884</td>
<td>1,1,1,2,3,4,4,5,5,5-Decafluoropentane techn., ~80% (GC)</td>
<td>C₁₀F₁₄</td>
<td>252.06</td>
<td>100 ml; 500 ml</td>
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<tr>
<td>77273</td>
<td>PerfluorohexaneFC-72purum, mixture of isomers, assay of perfluoro-n-hexane: ~85%</td>
<td>C₆F₁₄</td>
<td>338.04</td>
<td>10 ml; 50 ml</td>
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<tr>
<td>37,924-7</td>
<td>Perfluorohexane contains perfluorocyclohexane and ~5% perfluoropentane, 95%</td>
<td>C₆F₁₄</td>
<td>338.04</td>
<td>10 ml; 50 ml</td>
</tr>
<tr>
<td>77272</td>
<td>Perfluoroheptane pract., mixture of isomers, assay of perfluoro-n-heptane: ~80%</td>
<td>C₇F₁₄</td>
<td>388.05</td>
<td>10 ml; 50 ml</td>
</tr>
<tr>
<td>35,923-8</td>
<td>Octadecfluorooctane 98.0%</td>
<td>C₁₉F₁₈</td>
<td>438.06</td>
<td>25 g; 100 g</td>
</tr>
<tr>
<td>77286</td>
<td>Octadecafluoroctane Fraction purum, ≥97.0% (GC)</td>
<td>Perfluoroctane fraction (~70% Perfluoroctane)</td>
<td>488.07</td>
<td>10 ml; 50 ml; 250 ml</td>
</tr>
<tr>
<td>40,641-4</td>
<td>Perfluorononane 98.0%</td>
<td>C₁₀F₁₈</td>
<td>488.07</td>
<td>5 ml; 25 ml</td>
</tr>
</tbody>
</table>

*New offerings are added monthly, so don’t hesitate to contact your local Sigma-Aldrich Office (see back cover) when you cannot find the product you are looking for! For additional technical information, please contact your local Technical Services Department (see back cover) or visit our web-site at [www.sigma-aldrich.com/fluka](http://www.sigma-aldrich.com/fluka)*
### Solvents continued

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<th>Formula</th>
<th>Mass</th>
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<tr>
<td>13,393-0</td>
<td>Dodecafluorocyclohexane</td>
<td>C₁₂F₁₈</td>
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<tr>
<td>77280</td>
<td>(Trifluoromethyl)undecafluorocyclohexane purum, ~97% (GC)</td>
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<td>350.06 M</td>
<td>25 ml; 100 ml; 250 ml</td>
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<td>77268</td>
<td>Hexadecafluoro-1,3-dimethylcyclohexane techn., ~80% (GC)</td>
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<td>400.06 M</td>
<td>50 ml</td>
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<tr>
<td>53,535-4</td>
<td>Perfluoro-1,2-dimethylcyclohexane mixture of isomers, 98%</td>
<td>C₁₅F₁₈</td>
<td>400.06 M</td>
<td>5 ml; 25 ml</td>
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<td></td>
<td>Hexadecafluoro-1,2-dimethylcyclohexane</td>
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<td>416.06 M</td>
<td>1 g; 5 g</td>
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<td>78744</td>
<td>Hexadecafluoro-2-butyltetrahydrofuran purum p.a.</td>
<td>C₁₅F₁₈O</td>
<td>416.06 M</td>
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<tr>
<td>77264</td>
<td>Octadecafluorodecahydronaphthalene pract.(cis+trans), ~95% (GC)</td>
<td>C₂₀F₁₈</td>
<td>462.08 M</td>
<td>10 ml; 50 ml; 250 ml</td>
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<tr>
<td>37,243-9</td>
<td>Perfluoromethyldecalin) mixture of isomers, tech. 80%</td>
<td>C₁₅F₁₈</td>
<td>512.09 M</td>
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<td>52506</td>
<td>Hexafluorobenzene for NMR-spectroscopy ≥99.5% (GC)</td>
<td>C₆F₆</td>
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<td>(Trifluoromethyl)-benzene purum, ≥98.0% (GC)</td>
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<td>146.11 M</td>
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<tr>
<td>77299</td>
<td>Heptacosfluorotributylamine puriss., p.a</td>
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<td>77306</td>
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<td>371.05 M</td>
<td>5 ml; 25 ml</td>
</tr>
</tbody>
</table>

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AVAILABLE FIRST QUARTER 2002:
Starter Kit ‘C-C coupling with FPOS technology

Sigma-Aldrich is committed to introduce promising new technologies in Organic Synthesis! Explore soon the benefits of FBC-technology in one of the most important synthetic fields:

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The new Fluka Fluorous Biphase Catalysis, Kit I: C-C-Coupling will contain perfluorotagged Pd-catalyst and solvents to run up to 10 catalytic reactions under fluorous biphasic conditions. Furthermore, the catalyst can be recycled and reused for several additional runs.

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While the book is extensively indexed by product name (50,000 index entries) and molecular formula, this CD-ROM version has huge advantages of electronic access. An easy search for the full text using any character string, results in fast, efficient access to the data in ways that are simply not possible with the printed version.

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What is Phase Transfer Catalysis?
As the chemical industry strives to improve process efficiency, safety and reduce environmental impact, Phase Transfer Catalysis (PTC) has become recognized as a useful tool to achieve these goals.

The PTC methodology involves a substrate (which is soluble in the organic layer) and an anionic reagent (often a nucleophile), which is dissolved in the aqueous layer. The substrate and the anion are then brought together by a catalyst, which transports the anion into the organic phase where reaction can take place with the substrate.

Quaternary ammonium and phosphonium salts with their unique capability to dissolve in both aqueous and organic liquids are the catalysts of choice for most phase transfer applications. The ammonium derivatives are the most commonly used, but the phosphonium based phase transfer catalysts offer other interesting properties as well, like higher thermal stability. Other phase transfer catalysts include crown ethers and polyethyleneglycols (PEG).

What are its applications?
Some examples of well-known phase transfer catalyzed reactions include:

- Nucleophilic substitution reactions, like halogenations and cyanations,
- Alkylation and condensation reactions
- Oxidations and reductions
- Elimination reactions
- Wittig and Wittig-Horner reactions

What is the advantage as compared to other systems?
There are several advantages of the phase transfer catalysis system over single-phase systems, such as:

- An increased reaction rate
- A lower reaction temperature
- Avoiding the need for expensive anhydrous or aprotic solvents.
- The use of water together with an organic solvent as reaction medium.

Interestingly, some reactions are known to occur in a PTC-system that do not work in a normal system. The efficiency of phase transfer catalysis is influenced by the bulkiness of the groups attached to the phase transfer catalyst, its lipophilicity as well as that of its counter ion. For this reason Fluka offers a broad range of ammonium, phosphonium- and polyether-based phase transfer catalysts, from which we are proud to present you a selection below.

FOR A COMPLETE LISTING OF THE BROAD RANGE OF PHASE TRANSFER CATALYSIS REAGENTS, PLEASE CHECK OUT OUR Fluka/Riedel-de-Haën Catalog 2001-2002

Ready to scale up? For larger quantities, contact your local Sigma-Aldrich Office or visit our web site at www.sigma-aldrich.comsafc
### Ammonium based PTC Reagents

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<tr>
<td>86860</td>
<td>Tetrabutylammonium bromide puriss., ≥99.0% (AT)</td>
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<td>M₄₅₂.38</td>
<td>[1643-19-2]</td>
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<td>M₄₅₂.38</td>
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<td>50 g</td>
<td>250 g</td>
<td>1 kg</td>
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<tr>
<td>86870</td>
<td>Tetrabutylammonium chloride purum, ≥97.0% (AT)</td>
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<td>M₂₇₇.92</td>
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<tr>
<td>86872</td>
<td>Tetrabutylammonium fluorido trihydrate purum, ≥97.0% (NT)</td>
<td>C₂₅H₅₂F₃O₃</td>
<td>M₅₁₉.₅₂</td>
<td>[87749-50-6]</td>
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<td>10 g</td>
<td>50 g</td>
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<tr>
<td>86843</td>
<td>Tetrabutylammonium fluorido trihydrate pract., ~95% (T)</td>
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<td>M₅₁₉.₅₂</td>
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<td>50 g</td>
<td>250 g</td>
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<tr>
<td>86900</td>
<td>Tetrabutylammonium fluorido solution purum, ~1 M in THF</td>
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<td>M₃₂₆.₄₇</td>
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<td>86875</td>
<td>Tetrabutylammonium hydrogen sulfate purum, ≥97.0% (T)</td>
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<td>86894</td>
<td>Tetrabutylammonium iodide purum, ≥98.0% (AT)</td>
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<td>M₃₆₉.₃₈</td>
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<td>86886</td>
<td>Tetrabutylammonium thiocyanate purum, ≥99.0% (AT)</td>
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<td>M₃₀⁰.₅₅</td>
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<tr>
<td>86873</td>
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<td>M₃₂₉.₂₈</td>
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<td>13952</td>
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<td>M₂₃₀.₁₆</td>
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<td>M₁₈₅.₇₀</td>
<td>[5₆₉₃-9]</td>
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<th>Purity</th>
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<tbody>
<tr>
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<td>Hexadecyltrimethylammonium bromide purum, ~98% (AT)</td>
<td>C₁₅H₃₃BrN</td>
<td>M₃₆₄.₄₆</td>
<td>[₅₇-0₉-0]</td>
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<td>52366</td>
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<td>Hexadecyltrimethylammonium chloride solution pract., ~25% in water</td>
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<td>[1₁₂-₀₂-7]</td>
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<td>52373</td>
<td>Hexadecyltrimethylammonium hydrogen sulfate purum, ≥97.0% (T)</td>
<td>C₁₅H₃₃NO₃S</td>
<td>M₃₈₁.₆₁</td>
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<td>5 g</td>
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<tr>
<td>69486</td>
<td>Methyltributylcarbinol chloride bromide purum, ≥98.0% (AT)</td>
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<td>[₅₁₃₇-₅₅-₃]</td>
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</table>

*Fluka is proud to present a broad selection of PTC Reagents. For a full range of our products, visit our web site at [www.sigma-aldrich.com/fluka](http://www.sigma-aldrich.com/fluka)*
## Ammonium based PTC Reagents continued

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<th>Formula</th>
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<th>CAS Registry</th>
<th>Quantity</th>
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<td>210.16</td>
<td>71-91-0</td>
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<td>165.70</td>
<td>56-34-8</td>
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<td>Tetraethylammonium fluoride dihydrate</td>
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<td>185.28</td>
<td>665-46-3</td>
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<td>86627</td>
<td>Tetraethylammonium hexafluorophosphate</td>
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<td>Tetraethylammonium tetrafluoroborate</td>
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## Phosphonium based PTC Reagents

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<td>507.67</td>
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<td>86919</td>
<td>Tetrabutylphosphonium chloride</td>
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<td>294.89</td>
<td>2304-30-5</td>
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<td>Tetrabutylphosphonium bromide</td>
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<td>339.34</td>
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## Crown ethers and PEG based PTC Reagents

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<td>294-93-9</td>
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<td>28123</td>
<td>15-Crown-5</td>
<td>C&lt;sub&gt;H&lt;/sub&gt;&lt;sub&gt;15&lt;/sub&gt;O&lt;sub&gt;4&lt;/sub&gt;</td>
<td>220.20</td>
<td>33100-27-5</td>
<td>5 ml; 25 ml</td>
</tr>
<tr>
<td>33531</td>
<td>Dibenzo-18-crown-6</td>
<td>C&lt;sub&gt;H&lt;/sub&gt;&lt;sub&gt;2&lt;/sub&gt;&lt;sub&gt;O&lt;/sub&gt;&lt;sub&gt;4&lt;/sub&gt;</td>
<td>360.41</td>
<td>14187-32-7</td>
<td>5 g; 25 g</td>
</tr>
<tr>
<td>33539</td>
<td>Dibenzo-24-crown-8</td>
<td>C&lt;sub&gt;H&lt;/sub&gt;&lt;sub&gt;2&lt;/sub&gt;&lt;sub&gt;O&lt;/sub&gt;&lt;sub&gt;4&lt;/sub&gt;</td>
<td>448.52</td>
<td>14174-09-5</td>
<td>1 g; 5 g</td>
</tr>
<tr>
<td>28125</td>
<td>18-Crown-6</td>
<td>C&lt;sub&gt;H&lt;/sub&gt;&lt;sub&gt;2&lt;/sub&gt;&lt;sub&gt;O&lt;/sub&gt;&lt;sub&gt;4&lt;/sub&gt;</td>
<td>264.32</td>
<td>17455-13-9</td>
<td>5 g; 25 g; 100 g</td>
</tr>
<tr>
<td>36665</td>
<td>Dicyclohexano-18-crown-6</td>
<td>C&lt;sub&gt;H&lt;/sub&gt;&lt;sub&gt;30&lt;/sub&gt;O&lt;sub&gt;4&lt;/sub&gt;</td>
<td>372.51</td>
<td>16069-36-6</td>
<td>1 g; 5 g; 25 g</td>
</tr>
<tr>
<td>36668</td>
<td>Dicyclohexano-24-crown-8</td>
<td>C&lt;sub&gt;H&lt;/sub&gt;&lt;sub&gt;42&lt;/sub&gt;O&lt;sub&gt;4&lt;/sub&gt;</td>
<td>460.61</td>
<td>17455-23-1</td>
<td>1 ml; 5 ml</td>
</tr>
</tbody>
</table>

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### Crown ethers and PEG based PTC Reagents

<table>
<thead>
<tr>
<th>Code</th>
<th>Name</th>
<th>Formula</th>
<th>Mol. Wt.</th>
<th>CAS</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>93373</td>
<td>Tris[2-(2-methoxyethoxy)ethyl]amine</td>
<td>C₉H₂₇NO₃</td>
<td>M=323.43</td>
<td>[70384-51-9]</td>
<td>25 ml; 100 ml</td>
</tr>
<tr>
<td>52910</td>
<td>4,7,13,16,21,24-Hexaoxa-1,10-diazabicyclo[8.8.8]hexacosane</td>
<td>C₇₄H₁₄₂N₂O₁₂</td>
<td>M=376.50</td>
<td>[23978-09-8]</td>
<td>250 mg; 1 g</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Code</th>
<th>Name</th>
<th>Formula</th>
<th>Mol. Wt.</th>
<th>CAS</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>81150</td>
<td>Polyethylene glycol 200 purum</td>
<td>M=190-210</td>
<td></td>
<td>[25322-68-3]</td>
<td>1 l, 5 l</td>
</tr>
<tr>
<td>81170</td>
<td>Polyethylene glycol 400 purum</td>
<td>M=380-400</td>
<td></td>
<td>[25322-68-3]</td>
<td>1 l, 5 l</td>
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<tr>
<td>81180</td>
<td>Polyethylene glycol 600 purum</td>
<td>M=570-630</td>
<td></td>
<td>[25322-68-3]</td>
<td>1 kg, 5 kg</td>
</tr>
<tr>
<td>81190</td>
<td>Polyethylene glycol 1000 purum</td>
<td>M=570-630</td>
<td></td>
<td>[25322-68-3]</td>
<td>1 kg, 5 kg</td>
</tr>
</tbody>
</table>

### PTC based reagents on Polymer Support

<table>
<thead>
<tr>
<th>Code</th>
<th>Name</th>
<th>Formula</th>
<th>Mol. Wt.</th>
<th>CAS</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>90806</td>
<td>Tributylmethylammonium chloride polymer bound</td>
<td>Cl₃(CH₂)₃N⁺Cl⁻</td>
<td></td>
<td></td>
<td>5 g; 25 g</td>
</tr>
<tr>
<td>53265</td>
<td>Hexyltributylphosphonium bromide on polymer support</td>
<td>Cl₃(CH₂)₃P⁺Br⁻</td>
<td></td>
<td></td>
<td>5 g; 25 g</td>
</tr>
<tr>
<td>90808</td>
<td>Tributylmethylphosphonium chloride polymer bound</td>
<td>Cl₃(CH₂)₃P⁺Cl⁻</td>
<td></td>
<td></td>
<td>5 g; 25 g</td>
</tr>
<tr>
<td>52735</td>
<td>Hexamethylophosphoramide polymer bound</td>
<td>Cl₃(CH₂)₃N⁺Cl⁻</td>
<td></td>
<td></td>
<td>5 g</td>
</tr>
<tr>
<td>81185</td>
<td>Polyethylene glycol 600 monobenzyl ether polymer bound</td>
<td>Cl₃(CH₂)₃N⁺Cl⁻</td>
<td></td>
<td></td>
<td>1 g; 5 g</td>
</tr>
<tr>
<td>81317</td>
<td>Polyethylene glycol 750 monobenzyl monomethyl ether polymer bound</td>
<td>Cl₃(CH₂)₃N⁺Cl⁻</td>
<td></td>
<td></td>
<td>10 g; 50 g</td>
</tr>
</tbody>
</table>

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