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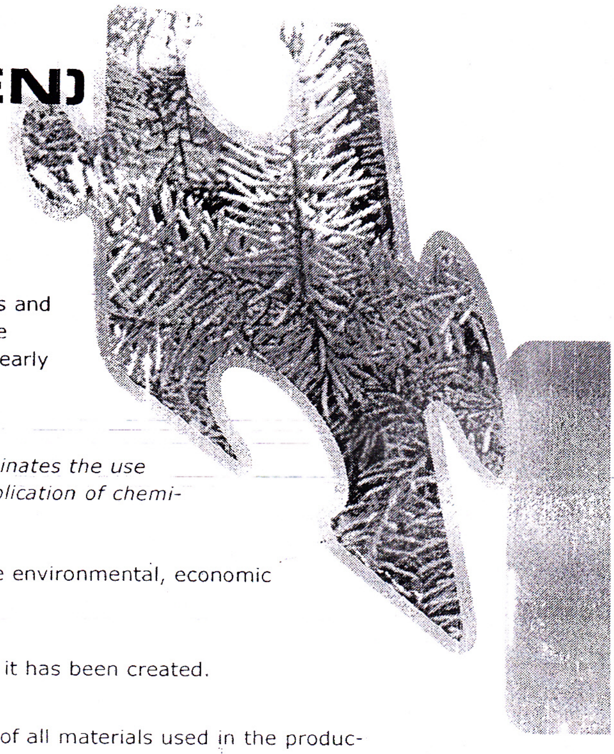
SUSTAINABLE (GREEN) CHEMISTRY GREEN SOLVENTS



Growing awareness of the environmental consequences of chemical products and the processes by which they are produced has led to the development of the concept of "Sustainable (Green) Chemistry" in the United States during the early nineties.

The definition given by its founder, Paul T. Anastas, is the following:
"Green Chemistry is the utilization of a set of principles that reduces or eliminates the use and generation of hazardous substances in the design, manufacture and application of chemical products."

It is based on the following **12 principles**, which take into consideration the environmental, economic and safety aspects of chemistry:

1. **Prevention**
   It is better to prevent waste rather than treat or clean up waste after it has been created.
2. **Atom Economy**
   Synthetic methods should be designed to maximize the incorporation of all materials used in the production of the final product.
3. **Less Hazardous Chemical Syntheses**
   Synthetic methods should be designed to use or generate substances that have little or no toxicity to human health and the environment.
4. **Designing Safer Chemicals**
   Chemical products should be designed to perform the expected function while minimizing their toxicity.
5. **Safer Solvents and Auxiliaries**
   The use of auxiliary substances, such as solvents or separation agents, should be avoided as much as possible and, if employed, innocuous when used.
6. **Design for Energy Efficiency**
   The energy requirements of chemical processes should be minimized and recognized for their environmental and economic impacts. If possible, synthetic methods should be conducted at ambient temperature and pressure.
7. **Use of Renewable Raw Materials**
   A raw material or feedstock should be renewable rather than non-renewable, as far as technically and economically feasible.
8. **Reduce Derivatives**
   Unnecessary derivatization should be minimized or avoided if possible, since these steps can produce waste.
9. **Catalysts**
   Catalytic reagents, as selective as possible, are preferable to stoichiometric reagents.
10. **Design for Degradation**
    Chemical products should be designed so that at the end of their life cycle they break down into innocuous degradation products and do not persist in the environment.
11. **Real-time Analysis for Pollution Prevention**
    Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control prior to the formation of hazardous substances.
12. **Inherently Safer Chemistry for Accident Prevention**
    The substances used in a chemical process should be selected to minimize the risk of chemical accidents, including releases, explosions and fires.

Green Chemistry

In the interest of Green Chemistry, Carlo Erba Reagenti offers the following solvents:

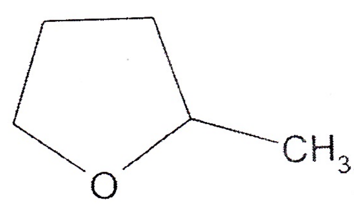
- 2-Methyltetrahydrofuran (MeTHF)
- Cyclopentyl Methyl Ether (CPME)
- N,N'-Dimethylpropyleneurea (DMPU)
- 1,3-Propanediol
- 1,3-Dioxolane
- Ionic solvents

These solvents have the following characteristics vs. those of some common solvents:

	Alternative solvents					Some classical solvents				
Solvent	**MeTHF**	**CPME**	**DMPU**	**1,3-propane-diol**	**1,3-diox-olane**	**DMF**	**THF**	**Et_2O**	**Dioxane**	**CH_2Cl_2**
Molecular weight (g/mol)	86,14	100,16	128,18	76,1	74,08	73,095	72,108	74,124	88,107	84,933
Density (20°C)[g/cm3]	0,85	0.86	1,06	1,053	1,067	0,95	0.89	0.71	1.03	1,32
Boiling point [°C]	80	106	246	214	75,6	153	65	34.6	101	39,6
Melting point [°C]	-136	<-140	-23	-26,7	-95	-61	-108.5	-116.3	11.8	-97
Flash point [°C]	-11	-1	120	129	-6	58	-14.5	-45	12	-
Viscosity (20°C)[cP]	0,6 (25°C)	0.55	-	0,52	0,6 (25°C)	0,802	0.55	0.2448	1.31	0,43
n (refractive index) (20°C)	1,406	1,4189	-	1,4386	1,3974	1,42	1,407	1,353	1,422	1,42
Dielectric constant (25°C)	7	4.76	-	-	7,34	-	7.58	4.197	2.227	11
Azeotropic point with water [°C]	71	83(*)	-	-	71 (*)	-	64	34.2	87.8	-
Solubility in water (23°C)[g/100g]	14	1.1	-					6.5		1,32
Solubility of water in the solvent (23°C)[g/100g]	4,4	0.3	-					1.2		0,14
Explosion range [vol%] (limite inferiore)	1,5	1.1	-	2,6	2,1	2,2	1.84	1.85	2	13
Explosion range [vol%] (limite superiore)	8,9	9.9	-	16,6	20,5	16	11.8	48	22	22

- azeotropic composition: CPME 83.7/water 16.3 (wt%)
  organic phase: CPME 98.9/water 1.1 (wt%)
  aqueous phase: CPME 0.78/water 99.22 (wt%)
  aqueous phase: Dioxolane 93%

2-Methyltetrahydrofuran (2MeTHF)



2MeTHF represents an excellent alternative to tetrahydrofuran. It is derived from renewable sources and guarantees superior versatility, efficiency and reactivity in Grignard and organometallic reactions. It is an aprotic solvent which is not miscible with water, particularly suited for reactions in biphasic environments, such as amidations and nucleophilic substitutions.

Improvements of 2MeTHF over THF:

- Higher boiling point --> allows higher reaction temperatures
- Lower solubility in water --> allows improved performance in biphasic reactions and simplifies recovery and anhydrification
- Better ecocompatibility --> it is obtained from renewable sources, while THF is a petroleum derivative
- It is non-irritating to the eyes and respiratory tract

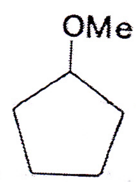
Specifications

Parameter	Units	Special grade for HPLC	Technical Grade for Synthesis
Titer (GC)	%	> 99.5	> 99
Color	Hazen	< 10	
Water content (K.F.)	mg/kg	< 200	< 300
Non-volatile residue	mg/kg	< 5	
Peroxides (H_2O_2)	mg/kg	< 300	< 100
UV transmittance (1cm- ref : water)			
at 240 nm	%	> 30	
at 250 nm	%	> 50	
at 260 nm	%	> 70	
at 280 nm	%	> 90	
> 310 nm	%	> 98	
Stabilizer (BHT)	mg/kg	not stabilized	150 - 400

Available formats

Product	Package	Size	Code
2-Methyltetrahydrofuran, **Special Grade** for HPLC	Glass	1000 ml	P9963716
	Glass	2500 ml	P9963721
2-Methyltetrahydrofuran, **Technical Grade** for Synthesis	Glass	1000 ml	P9960216
	Plastic drum	5000 ml	P9960229
	Metal drum	25 liters	P9960248
	Metal drum	200 liters	P9960268

Cyclopentyl Methyl Ether (CPME)



CPME is a solvent characterized by a high boiling point, low tendency towards the formation of peroxides and relative stability in acid and basic environments. These properties make it a valid alternative to other ether solvents such as methyl tert-butyl ether, dioxane, diethyl ether, tetrahydrofuran and 1,2-dimethoxyethane. It is a hydrophobic solvent which is particularly suitable for organometallic reactions.

Improvements of CPME over other ethers:

- Greater stability in acid and basic environments --> allows greater variability in the reaction conditions
- Higher boiling point --> allows higher reaction temperatures
- Limited solubility in water (1.1/100g at 23°C) --> improved performance in biphasic reactions and simplified recovery
- Low volatility --> less solvent loss
- Greater peroxide formation stability --> prevents the formation of subproducts

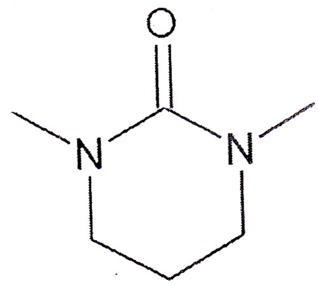
Specifications

Parameter	Units	Technical Grade for Synthesis
Titer (GC)	%	> 99.9
Color	Hazen	< 10
Water content (K.F.)	mg/kg	< 100
Peroxides (H_2O_2)	mg/kg	< 50

Available formats

Product	Package	Size	Code
Cyclopentyl Methyl Ether, **Technical Grade** for Synthesis	Glass	1000 ml	P8010216
	Plastic drum	5000 ml	P8010229
	Metal drum	25 liters	P8010248
	Metal drum	200 liters	P8010268

N,N'-Dimethylpropyleneurea (DMPU)



DMPU is a solvent that can be used in place of dimethylformamide due to its special characteristics: aproticity, polarity and unique performance in SN2 nucleophilic substitutions. These properties make it particularly suitable for synthesis processes, in the industry sector as well as the laboratory.

Specifications

Parameter	Units	Technical Grade for Synthesis
Titer (GC)	%	> 99
Water content (K.F.)	mg/kg	< 1000

Available formats

Product	Package	Size	Code
N,N'-Dimethylpropyleneurea, **Technical Grade** for Synthesis	Glass	1000 ml	P8020216
	Plastic drum	5000 ml	P8020229
	Metal drum	25 liters	P8020248
	Metal drum	200 liters	P8020268

1,3-Propanediol

1,3-Propanediol is a product obtained from a renewable source (corn) with characteristics and performance comparable to petroleum derivative solvents.
It offers the advantages of biodegradability, low toxicity and greater thermal stability with respect to other glycols and ethylene glycols. It is used in polyester resin manufacturing, urethane chemistry and the production of antifreezes and heat transfer fluids.

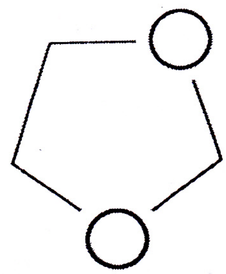
Specifications

Parameter	Units	Technical Grade for Synthesis
Titer (GC)	%	> 99.70
Water content (K.F.)	mg/kg	< 1000

Available formats

Product	Package	Size	Code
1,3-Propanediol, **Technical Grade** for Synthesis	Glass	1000 ml	P8040216
	Plastic drum	5000 ml	P8040222
	Plastic drum	25 liters	P8040249
	Metal drum	200 liters	P8040268

1,3-Dioxolane



The physical, chemical and toxicological properties of 1,3-dioxolane enable it to be considered a solvent as well as a reagent. It can be used as an alternative to dichloromethane, dichloroethane and methyl ethyl ketone, under neutral or basic reaction conditions, or in the place of THF and DMSO.
It is used in organic chemistry, the polymer industry, as a copolymerizing agent and in the paint industry as a substitute for toluene and xylene.

Improvements of 1,3-dioxolane over other solvents:

- It is not carcinogenic, toxic, explosive or auto-flammable ' improved safety
- It has no unpleasant odor ' more convenient to use
- Low peroxide formation tendency ' prevents the formation of sub products
- Miscible in water and in most organic solvents ' allows greater variability in the reaction conditions

Specifications

Parameter	Units	Technical Grade for Synthesis
Titer (GC)	%	> 99.90
Water content (K.F.)	mg/kg	< 150
Peroxides (H_2O_2)	mg/kg	< 5
Stabilizer (BHT)	mg/kg	75

Available formats

Product	Package	Size	Code
1,3-Dioxolane, **Technical Grade** for Synthesis	Glass	1000 ml	P8030216
	Plastic drum	5000 ml	P8030222
	Plastic drum	25 liters	P8030249
	Metal drum	200 liters	P8030268

Ionic solvents

Ionic solvents are coordination compounds composed of organic cations and inorganic or organic anions. They have the property of being in the liquid state at temperatures below 100°C.
They are particularly suitable for organic synthesis, catalytic and enzymatic reactions, electrochemistry and delicate extractions of high-value products.

Characteristics

- non-volatile
- generally non-toxic
- non-flammable
- high thermal stability
- high reuse potential
- miscible or not in water depending on the nature of the anion
- high viscosity
- high conductivity
- high solvent power for organic and inorganic compounds
- "tailoring" - the solvent's properties can be changed significantly by changing the nature of the ions

Carlo Erba Reagenti offers its clients the possibility of requesting quotes on and ordering ionic solvents. Just send your request to the e-mail address chemicals@carloerbareagenti.com, specifying the product of interest and the volume requested.

SOLVENTS: PROPERTIES AND THEIR APPLICATIONS
IN GREEN CHEMISTRY

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In recent years, we are very interested in thermodynamics of green solvents and their applications green chemistry, which include mainly: 1)phase behavior and intermolecular molecular interaction in complex supercritical fluid (SCF), IL, supercritical (SC) CO2/IL and SC CO2/PEG systems; 2)chemical reactions in SC CO2, ILs and CO2/ILs, special attention is paid to enhancing the efficiency of chemical retractions using the unusual properties of green solvents; 3) the physicochemical properties and applications of the green microemulsions related with SC CO2, ILs and PEG; 4) fabrication and characterization of different functional materials using green solvents, including those that are difficult to prepare using conventional solvents. In this presentation, we will discuss some of our recent work.

New Solvent Systems Recyclable, True Green Chemistry

A research team at the University of Leicester, part of Leicester Green Chemistry Group, has developed novel solvent systems which are recyclable and environmentally compatible.
The team led by Drs. Andy Abbott and David Davies has developed a wide range of new ionic liquids made from simple precursors.

Ionic liquids have been studied extensively in recent years as they offer a potentially clean way to carry out chemical processes. They are non-volatile, while liquid over a wide range of temperatures, and offer a benign alternative to, for example, some strong acids.

In order to commercialize the technology, a joint venture company, Scionix Ltd, has been set up. It brings together the business and marketing skills of Genacys Ltd, a subsidiary of the Whyte Group Ltd., with the cross-disciplinary scientific skills of the team based at the University of Leicester.

These novel liquids can be used for a variety of applications including metal finishing (e.g., highly efficient chromium plating), catalysis (e.g., Friedel-Crafts reactions), batteries and metal recovery (e.g., waste-product reprocessing), among others.

Further benefits include limited sensitivity to water, readily available in large quantities and at comparable cost to many volatile organic solvents (VOS).

Until now, industrial uptake of ionic liquids has been limited by the extremely high cost of previous materials together with the moisture sensitivity and environmental incompatibility of aluminum-containing salts.

The Scionix team has shown (as recently published in Chemical Communications 2001, 2010-1) that mixtures of zinc chloride (found in some skin ointments and batteries) and choline chloride (a common additive to chicken feed) form non-volatile liquids at ambient temperatures.

These novel materials represent a cost reduction of more than one order of magnitude over previous ionic liquids.

Furthermore, as the use of VOS is environmentally hazardous, measures such as the Montreal protocol to limit the use of these solvents will necessitate the use of alternative solvent systems. Ionic liquids are now well placed to take advantage of the new marketplace.