

AcroSeal Packaging

An Application Guide



Solvents and Reagents
Drier For Longer

Introduction

Organic reagents have a wide series of applications in drug discovery, agrochemical research, flavours and fragrances, diagnostics and NMR analysis. Reactions often involve the use of air and moisture sensitive solvents, pyrophoric and hazardous reagents. Our AcroSeal™ packaging is an industry leading packaging solution for safe handling of these types of materials.

This brochure provides an overview of the key advantages of AcroSeal packaging for your research and outlines some important reactions that could benefit.

AcroSeal Packaging Provides...



PERFORMANCE

The specially designed multi-layer septum ensures a better re-seal thus minimizing atmospheric exposure and protecting the quality of your air and moisture sensitive solvents and reagents.



CONVENIENCE

A wide range of pre-prepared reagents in solution are available, reducing the risks and saving the time and effort of making your own.



SAFETY

Our AcroSeal cap system ensures you can transfer the contents of the bottle safely into your reaction vessel minimizing your exposure to potentially hazardous chemicals.



Contents

Page no.

| | |
|--|-----|
| Introduction | 2 |
| Performance | 3 |
| Grignard Reagents..... | 4 |
| Convenience..... | 5-6 |
| Organolithium Reagents..... | 7 |
| Safety | 8 |
| Hydride Reducing Reagents..... | 9 |
| Other AcroSeal Packaged Products | 10 |
| Top Tips for Using AcroSeal Packaging..... | 11 |



Performance

When carrying out synthetic organic chemistry, exposing many solvents and reagents to air and moisture inhibits their ability to perform properly and can cause some, if not all, of the following issues:

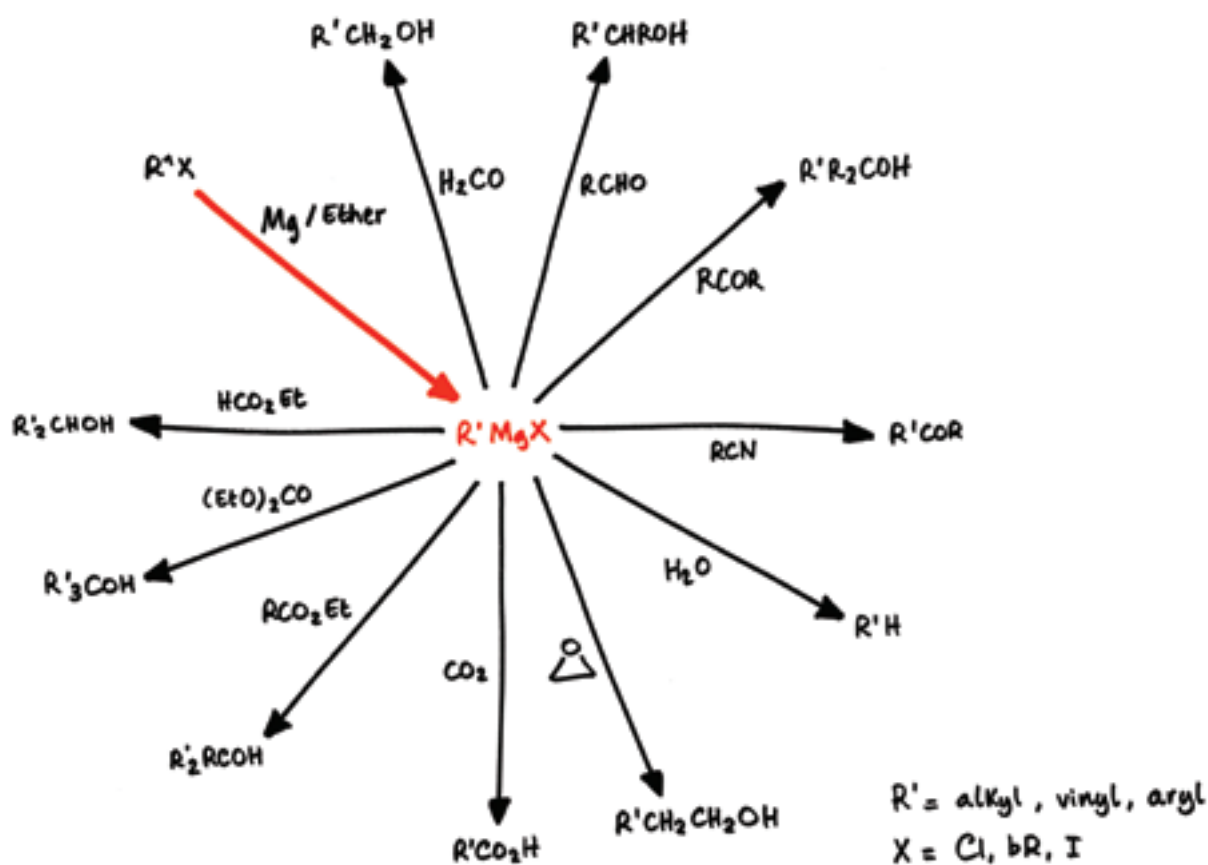
- A failed synthesis
- Poor yield
- Greater number of by-products/impurities
- More challenging purification

Our AcroSeal packaging solution is innovative and simple as we endeavour to:-

- Pack the product when it is as dry as possible
- Make it easy to keep it dry when transferring from the packaging into your dry system
- Ensure products stay dry between repeated use

Grignard Reaction

The Grignard reaction is an essential method in the formation of carbon-carbon bonds. In reactions involving Grignard Reagents it is essential to exclude water and air, which rapidly destroy the reagent. Therefore, we provide these sensitive reagents in the industry-leading AcroSeal packaging, preventing the degradation of the reagents. An example of a reaction that can be severely affected by the presence of water is the Grignard reaction.



Grignard Reactions

Grignard Reagents

A selection of our grignard reagents can be found in the table below.

| Product Code | Product Name | CAS no. |
|--------------|--|-------------|
| 20953 | Allylmagnesium bromide, 1M solution in diethyl ether, AcroSeal | 1730-25-2 |
| 20967 | Allylmagnesium chloride, 1.7M solution in THF, AcroSeal | 2622-05-1 |
| 38955 | Benzylmagnesium chloride, 1.4M solution in THF, AcroSeal | 6921-34-2 |
| 42746 | 3-Butenylmagnesium bromide, 0.5M solution in THF, AcroSeal | 7103-09-5 |
| 33167 | tert-Butylmagnesium chloride, 1.7M solution in THF, AcroSeal | 677-22-5 |
| 39749 | 3-Chlorophenylmagnesium bromide, 0.5M solution in THF, AcroSeal | 36229-42-2 |
| 44595 | Cyclopropylmagnesium bromide, 0.5M solution in 2-MeTHF, AcroSeal | 23719-80-4 |
| 39761 | Cyclopropylmagnesium bromide, 0.5M solution in THF, AcroSeal | 23719-80-4 |
| 43190 | (1,3-Dioxan-2-ylethyl)magnesium bromide, 0.5M solution in THF, AcroSeal | 480438-44-6 |
| 34729 | Ethylmagnesium bromide, 3M in diethyl ether, AcroSeal | 925-90-6 |
| 21047 | Ethylmagnesium bromide, 0.9M solution in THF, AcroSeal | 925-90-6 |
| 25257 | Ethylmagnesium chloride, 2.7M (25 wt.%) solution in THF, AcroSeal | 2386-64-3 |
| 43912 | Ethynylmagnesium bromide, 0.5M solution in THF, AcroSeal | 4301-14-8 |
| 38895 | Ethynylmagnesium chloride, 0.6M solution in THF/Toluene, AcroSeal | 65032-27-1 |
| 43303 | Heptylmagnesium bromide, 1M solution in diethyl ether, AcroSeal | 13125-66-1 |
| 42775 | Isopropenylmagnesium bromide, 0.5M solution in THF, AcroSeal | 13291-18-4 |
| 42678 | Isopropylmagnesium bromide, 3M solution in 2-MeTHF, AcroSeal | 920-39-8 |
| 21285 | Isopropylmagnesium chloride, 2.0M solution in THF, AcroSeal | 1068-55-9 |
| 38628 | Isopropylmagnesium chloride - Lithium chloride complex, 1.3M solution in THF, AcroSeal | 745038-86-2 |
| 21073 | 2-Mesitylmagnesium bromide, 1M solution in THF, AcroSeal | 2633-66-1 |
| 37742 | 4-Methoxyphenylmagnesium bromide, 1M solution in THF, AcroSeal | 13139-86-1 |
| 42741 | 2-Methylallylmagnesium chloride, 0.5M solution in THF, AcroSeal | 5674-01-1 |
| 18354 | Methylmagnesium bromide, 3M solution in diethyl ether, AcroSeal | 75-16-1 |
| 39112 | Methylmagnesium bromide, 3.2M solution in 2-MeTHF, AcroSeal | 75-16-1 |
| 37738 | Methylmagnesium bromide, 1M solution in THF, AcroSeal | 75-16-1 |
| 25256 | Methylmagnesium chloride, 3M (22 wt.%) solution in THF, AcroSeal | 676-58-4 |
| 42740 | Methylmagnesium iodide, 3M solution in diethyl ether, AcroSeal | 917-64-6 |
| 43556 | 2-Methyl-1-propenylmagnesium bromide, 0.5M solution in THF, AcroSeal | 38614-36-7 |
| 43874 | Pentafluorophenylmagnesium bromide, 0.5M solution in diethyl ether, AcroSeal | 879-05-0 |
| 43467 | 1-Propenylmagnesium bromide, 0.5M solution in THF, AcroSeal | 14092-04-7 |
| 42607 | 1-Propynylmagnesium bromide, 0.5M solution in THF, AcroSeal | 16466-97-0 |
| 37746 | (Trimethylsilyl)methylmagnesium chloride, 1.3M solution in THF, AcroSeal | 13170-43-9 |
| 44597 | Vinylmagnesium bromide, 1M solution in 2-MeTHF, AcroSeal | 1826-67-1 |
| 20939 | Vinylmagnesium bromide, 0.7M solution in THF, AcroSeal | 1826-67-1 |
| 25259 | Vinylmagnesium chloride, 1.9M (16.5 wt.%) solution in THF, AcroSeal | 3536-96-7 |

Full product listing and pack sizes available online [acros.com](https://www.acros.com)



Convenience

Freshly preparing anhydrous solvents and reagents for use in chemical synthesis is not a trivial exercise and takes time, specialized equipment and handling practices. For example, preparing gaseous solutions can involve handling cylinders and distillation.



Glove box to handle air and moisture sensitive reagents

Alkylolithium Reagents

The most common members of the alkylolithium family are n-Butyllithium, Methyllithium and tert-Butyllithium and these are widely used in organic synthesis. Fresh solutions can be created in the lab, requiring complex, potentially hazardous and time consuming steps, including movement and use of gas cylinders and distillation steps.

Alternatively, AcroSeal packaging provides a wide range of anhydrous solvents and reagents for immediate use, saving you both time and money.

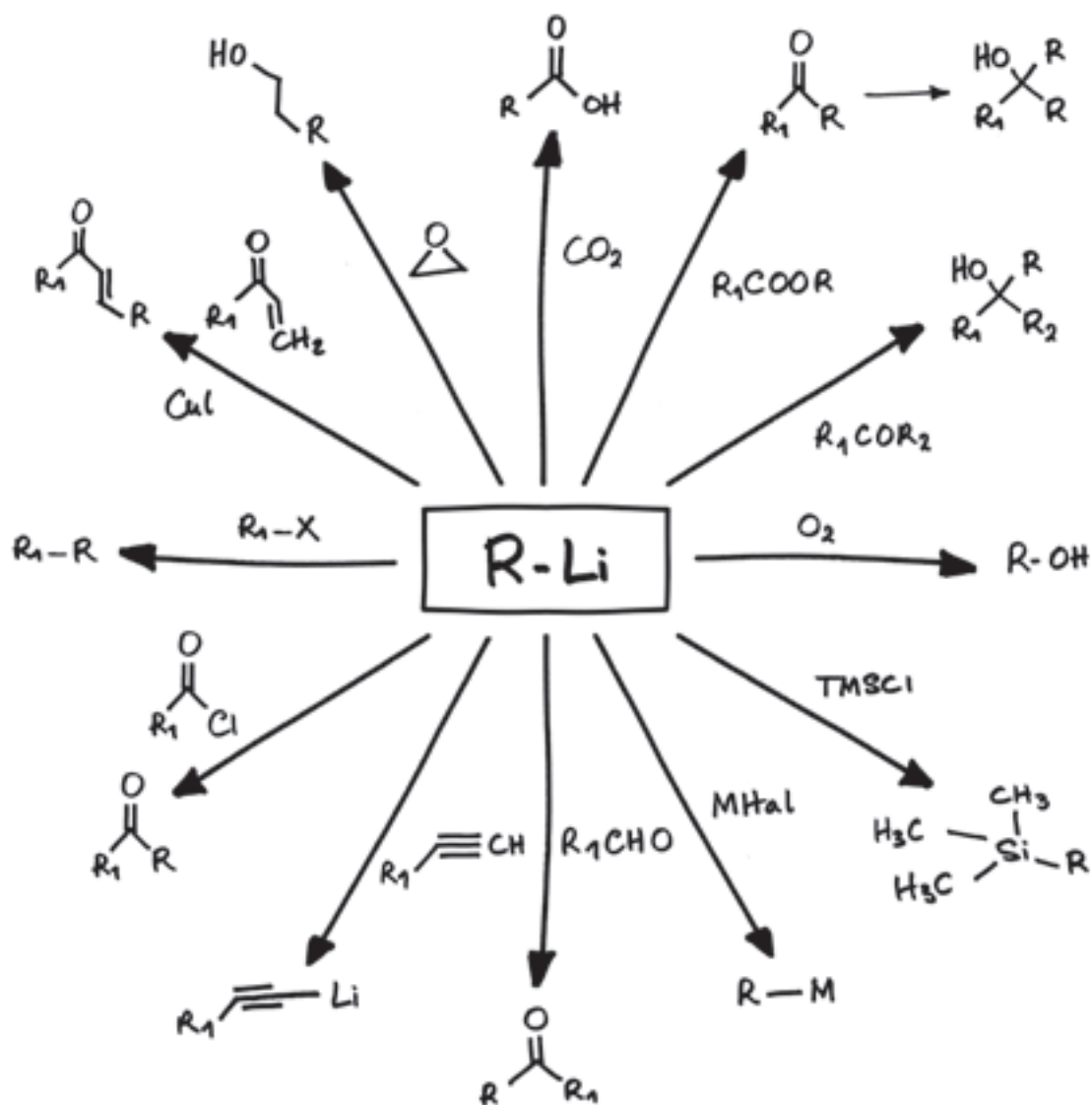
Some examples of their applications are given below:

- **Metallation** - Many hundreds of functionalised organolithium compounds have been prepared by the metallation reaction with n-Butyllithium or other alkylolithium compounds.
- **Ortho-metallation** - Metallation of an aromatic ring near a substituent, which acts as a "directed metalation group", is called ortho-metallation.
- **Nucleophilic Addition and Substitution** - Stabilized organolithium compounds like enolates and sulfonyl carbanions can react as nucleophiles with alkyl-halogenides and carbonyl compounds in a wide range of reactions:
 - Alkylation of Alkyl-halogenides
 - Addition to Carbonyl-compounds
 - Alkylation of Allyl-halogenides
 - Epoxide-Ring Opening
 - Conjugate Addition
 - Addition to Carbon dioxide



Convenience

- **Halogen-Metal Exchange** - The Halogen-metal exchange reaction was discovered in the late 1930s by Gilman and Wittig. The reaction is often used to prepare vinyl and aryllithium compounds from the more reactive alkyllithium species.
- **Transmetalation** - The organolithium compounds are very often used to prepare other metallorganic compounds through the transmetalation reaction.
- **Anionic Polymerisation** - A major industrial use of alkyllithium compounds, specifically n-Butyllithium, is the catalysis of the anionic polymerization of butadiene, isoprene and styrene.



Organolithium Reactions

Organolithium Reagents

A selection of our organolithium reagents can be found in the table below.

| Product Code | Product Name | CAS no. |
|--------------|--|-------------|
| 37749 | n-Butyllithium, 2.2M solution in cyclohexane, AcroSeal | 109-72-8 |
| 21335 | n-Butyllithium, 2.5M solution in hexanes, AcroSeal | 109-72-8 |
| 18127 | n-Butyllithium, 1.6M solution in hexanes, AcroSeal | 109-72-8 |
| 37893 | n-Butyllithium, 2.7M solution in toluene, AcroSeal | 109-72-8 |
| 18754 | sec-Butyllithium, 1.3M sol. in cyclohexane/hexane (92/8), AcroSeal | 598-30-1 |
| 39654 | tert-Butyllithium, 1.9M solution in pentane, AcroSeal | 594-19-4 |
| 44592 | tert-Butyllithium, 2M (18%) solution in heptane, AcroSeal | 594-19-4 |
| 30165 | n-Hexyllithium, 33 wt.% solution in n-hexane, AcroSeal | 21369-64-2 |
| 37759 | Isobutyllithium, 1.6M solution in heptane, AcroSeal | 920-36-5 |
| 43988 | Lithium acetylide ethylenediamine complex, 25 wt.% slurry in toluene, AcroSeal | 6867-30-7 |
| 43455 | Lithium aluminium hydride bis(tetrahydrofuran), 1M solution in toluene, AcroSeal | 123439-81-6 |
| 38023 | Lithium bis(trimethylsilyl)amide, 0.9M solution in methylcyclohexane, AcroSeal | 4039-32-1 |
| 34567 | Lithium bis(trimethylsilyl)amide, 1.0M sol. in methyl tert-butyl ether, AcroSeal | 4039-32-1 |
| 44611 | Lithium bis(trimethylsilyl)amide, 15% in 2-MeTHF/Ethylbenzene, AcroSeal | 4039-32-1 |
| 20955 | Lithium bis(trimethylsilyl)amide, 1M solution in THF, AcroSeal | 4039-32-1 |
| 34770 | Lithium bis(trimethylsilyl)amide, 1M solution in THF/Ethylbenzene, AcroSeal | 4039-32-1 |
| 44684 | Lithium tert-butoxide, 0.9M (8 wt.%) solution in 2-MeTHF, AcroSeal | 1907-33-1 |
| 37931 | Lithium tert-butoxide, 2.2M solution in THF, AcroSeal | 1907-33-1 |
| 26883 | Lithium diisopropylamide, 2M sol. in THF/n-heptane/ethylbenzene, AcroSeal | 4111-54-0 |
| 43287 | Lithium diisopropylamide mono(tetrahydrofuran), 1.5M solution in cyclohexane, AcroSeal | 123333-84-6 |
| 43362 | Lithium diphenylphosphide, 0.5M solution in THF, AcroSeal | 65567-06-8 |
| 38017 | Lithium ethoxide, 1M solution in ethanol, AcroSeal | 2388-07-0 |
| 39650 | Lithium isopropoxide, 3M solution in THF, AcroSeal | 2388-10-5 |
| 33675 | Lithium methoxide, pure, 2.2M (10 wt%) solution in methanol, AcroSeal | 865-34-9 |
| 38861 | Lithium phenoxide, 0.6M solution in THF, AcroSeal | 555-24-8 |
| 43350 | Lithium thiophenolate, 0.6M solution in THF, AcroSeal | 2973-86-6 |
| 17645 | Lithium tri-sec-butylborohydride, 1M solution in THF, AcroSeal | 38721-52-7 |
| 37758 | Lithium tri-tert-butoxyaluminumhydride, 1.1M solution in THF, AcroSeal | 17476-04-9 |
| 45069 | Lithium triethylborohydride, 1.7M solution in THF, AcroSeal | 22560-16-3 |
| 38065 | Lithium (trimethylsilyl)acetylide, 0.5M solution in THF/hexanes, AcroSeal | 54655-07-1 |
| 43911 | Lithium tris[(3-ethyl-3-pentyl)oxy]aluminumhydride, 0.5M solution in THF, AcroSeal | 79172-99-9 |
| 18875 | Methylolithium, 1.6 M sol. in diethyl ether (\pm 5% w/v), AcroSeal | 917-54-4 |
| 18129 | Methylolithium, 2.2M (6wt%) in diethyl ether with LiBr, AcroSeal | 332360-06-2 |
| 44584 | Methylolithium, 3% solution in 2-MeTHF/cumene, AcroSeal | 917-54-4 |
| 37745 | (Trimethylsilyl)methylolithium, 0.7M (10 wt%) solution in hexanes, AcroSeal | 1822-00-0 |

Full product listing and pack sizes available online [acros.com](https://www.acros.com)



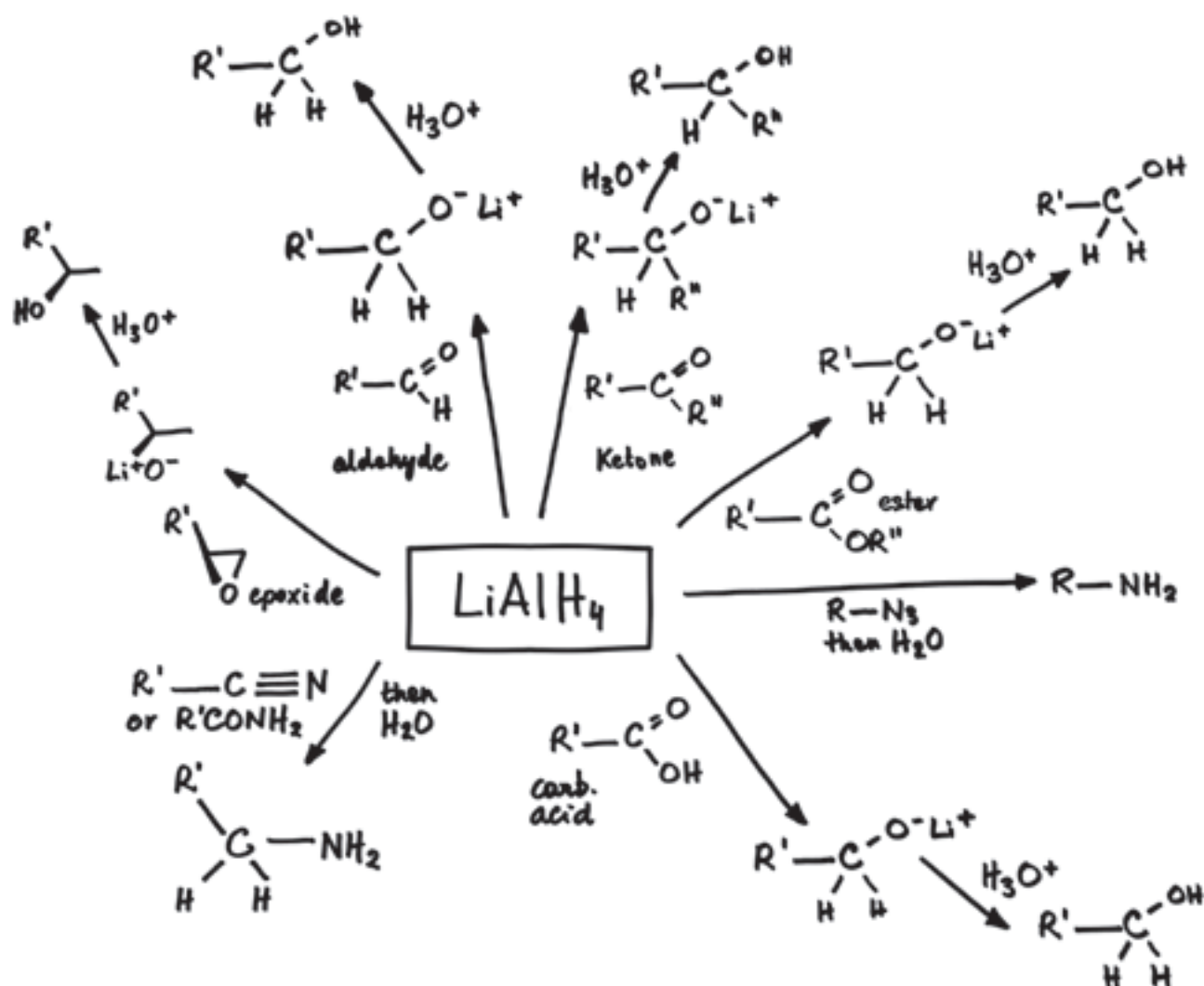
Safety

The highly reactive reagents often required in organic synthesis may be hazardous to use, including compounds that can be pyrophoric, toxic, carcinogenic, mutagenic, corrosive and odourous e.g. thiols.

AcroSeal packaging provides a safer solution for handling these reagents by allowing removal of the reagent from the bottle under an inert atmosphere and without exposure to the contents.

Lithium Aluminium Hydride

Lithium aluminium hydride is an example of an extremely pyrophoric reducing agent, used in organic synthesis, especially for the reduction of esters, carboxylic acids and amides.



Lithium Aluminium Hydride Reactions

Hydride Reducing Reagents

A selection of our hydride reducing reagents can be found in the table below.

| Product code | Product name | CAS no. |
|--------------|--|-------------|
| 20105 | Diisobutylaluminium hydride, 1.0M solution in heptane, AcroSeal | 1191-15-7 |
| 18379 | Diisobutylaluminium hydride, 1M solution in hexanes, AcroSeal | 1191-15-7 |
| 20103 | Diisobutylaluminium hydride, 1.1M solution in cyclohexane, AcroSeal | 1191-15-7 |
| 20108 | Diisobutylaluminium hydride, 1.2M (20 wt.%) solution in toluene, AcroSeal | 1191-15-7 |
| 19949 | Lithium aluminium hydride, 1M solution in THF, AcroSeal | 16853-85-3 |
| 37732 | Lithium aluminium hydride, 2.4M solution in THF, AcroSeal | 16853-85-3 |
| 38557 | Lithium aluminium hydride, 3.5M (15 wt.%) solution in toluene/THF, AcroSeal | 16853-85-3 |
| 19951 | Lithium aluminium hydride, 4.0M solution in diethyl ether, AcroSeal | 16853-85-3 |
| 43455 | Lithium aluminium hydride bis(tetrahydrofuran), 1M solution in toluene, AcroSeal | 123439-81-6 |
| 42888 | Lithium borohydride, 4M (10 wt.%) solution in THF, AcroSeal | 16949-15-8 |
| 37758 | Lithium tri-tert-butoxyaluminumhydride, 1.1M solution in THF, AcroSeal | 17476-04-9 |
| 17645 | Lithium tri-sec-butylborohydride, 1M solution in THF, AcroSeal | 38721-52-7 |
| 43911 | Lithium tris[(3-ethyl-3-pentyl)oxy]aluminumhydride, 0.5M solution in THF, AcroSeal | 79172-99-9 |
| 20968 | Lithium trisiamylborohydride, 1M solution in THF, AcroSeal | 60217-34-7 |
| 20547 | Potassium tri-sec-butylborohydride, 1M solution in THF, AcroSeal | 54575-49-4 |
| 18918 | Potassium triisopropoxyborohydride, 1M solution in THF, AcroSeal | 42278-67-1 |
| 43091 | Sodium bis(2-methoxyethoxy)aluminium hydride, 70 wt.% solution in toluene (approx. 3.5M), AcroSeal | 22722-98-1 |
| 19113 | Sodium borohydride, 0.5M solution in diglyme, AcroSeal | 16940-66-2 |
| 42913 | Sodium borohydride, 12% solution in 40% aq. NaOH solution, AcroSeal | 16940-66-2 |
| 37245 | Sodium cyanoborohydride, 1M solution in THF, AcroSeal | 25895-60-7 |
| 20003 | Sodium triethylborohydride, 1M solution in THF, AcroSeal | 17979-81-6 |
| 42914 | Sodium tri-sec-butylborohydride, 1M solution in THF, AcroSeal | 67276-04-4 |

Full product listing and pack sizes available online [acros.com](https://www.acros.com)

Other AcroSeal Packaged Products

Alongside the aforementioned categories of reagents, a broad range of other products are available packaged in AcroSeal, including:

- Deuterated solvents
- Extra dry solvents
- Organics
- Organometallics
- Reagents in solution

A selection of these reagents can be found in the tables below.

| Product code | Product name | CAS no. |
|-----------------------------|---|------------|
| Deuterated Solvents | | |
| 21742 | Acetonitrile-d ₃ , for NMR, 99.8 atom% D, AcroSeal | 2206-26-0 |
| 42677 | Chloroform-d, for NMR, 99.8 atom % D, AcroSeal | 865-49-6 |
| 42693 | Deuterium oxide, for NMR, 99.8 atom % D, AcroSeal | 7789-20-0 |
| 43399 | Dichloromethane-d ₂ , for NMR, 99.5 atom % D, AcroSeal | 1665-00-5 |
| 42694 | Methyl sulfoxide-d ₆ , for NMR, 99.9 atom% D, AcroSeal | 2206-27-1 |
| Extra Dry Solvents | | |
| 36431 | Acetonitrile, 99.9%, Extra Dry over Molecular Sieve, AcroSeal | 75-05-8 |
| 34846 | Dichloromethane, 99.8%, Extra Dry over Molecular Sieve, Stabilized, AcroSeal | 75-09-2 |
| 34843 | N,N-Dimethylformamide, 99.8%, Extra Dry over Molecular Sieve, AcroSeal | 68-12-2 |
| 34845 | Tetrahydrofuran, 99.5%, Extra Dry over Molecular Sieve, Stabilized, AcroSeal | 109-99-9 |
| 32697 | Tetrahydrofuran, 99.85%, Extra Dry, stabilized, AcroSeal | 109-99-9 |
| Organics | | |
| 42727 | Chlorodiisopropylphosphine, 96%, AcroSeal | 40244-90-4 |
| 44618 | N,N'-Diisopropylcarbodiimide, 99%, AcroSeal | 693-13-0 |
| 42720 | Pivaldehyde, 97%, AcroSeal | 630-19-3 |
| 43646 | Trioctylphosphine, 90%, technical grade, AcroSeal | 4731-53-7 |
| 44724 | Xylenes, 99%, for biochemistry and histology, mixed isomers with ethylbenzene, AcroSeal | 1330-20-7 |
| Organometallics | | |
| 30176 | Bis(cyclopentadienyl)dimethyltitanium, 5 wt% in toluene, AcroSeal | 1271-66-5 |
| 37756 | Diisobutylaluminium chloride, 0.8M solution in heptane, AcroSeal | 1779-25-5 |
| 18379 | Diisobutylaluminium hydride, 1M solution in hexane, AcroSeal | 1191-15-7 |
| 37724 | Dimethylzinc, 1.2M solution in toluene, AcroSeal | 544-97-8 |
| 18927 | Trimethylaluminium, 1.0M solution in heptane, AcroSeal | 75-24-1 |
| Reagents in Solution | | |
| 17706 | Borane-methyl sulfide complex, 94%, AcroSeal | 13292-87-0 |
| 17508 | Borane-tetrahydrofuran complex, 1M solution in THF, Stabilized, AcroSeal | 14044-65-6 |
| 17668 | Boron trichloride, 1M solution in methylene chloride, AcroSeal | 10294-34-5 |
| 38836 | Hydrogen chloride, 4N solution in 1,4-dioxane, AcroSeal | 7647-01-0 |
| 42879 | Potassium tert-butoxide, pure, 1.6-1.7M (20 wt.%) solution in THF, AcroSeal | 865-47-4 |

Full product listing and pack sizes available online [acros.com](https://www.acros.com)

Top Tips for Using AcroSeal Packaging

To get the best results using AcroSeal packaging, we recommend the following process:

1. Puncture the septum
2. Withdraw the required amount
3. Replace the nitrogen blanket
4. Store upright to prevent prolonged product contact with the seal

Advanced tips:

1. Prepare the nitrogen balloon in advance and use two balloons, one inside the other
2. Purge the doubled balloons with nitrogen three times before use
3. Bend the needle as it makes it easier to use and control
4. Flush each needle and syringe with nitrogen three times before use
5. Use the reaction flask to flush the syringe and needle prior to use



To get the best results from the septum, we recommend you use 18 to 21 gauge needles and puncture in a clock face pattern to avoid piercing the septum in the same place.

If you require a large amount of solvent remove the whole cap under an inert atmosphere and decant the desired amount of product from the bottle.

For further tips on how to use AcroSeal packaged products, view our demonstration video at [acros.com](https://www.acros.com).

In conclusion, AcroSeal packaging offers a superior advantage for your organic synthesis by providing quality products, saving you time and keeping you safer!



To view the full list of AcroSeal packaged products visit [acros.com](https://www.acros.com).

To place an order, contact your local Fisher Scientific office.



©2017 Thermo Fisher Scientific Inc. All rights reserved.
All other trademarks are the property of Thermo Fisher Scientific Inc. and its subsidiaries.

Credit to Dr Phil Helliwell, Teaching Laboratories Manager, Department of Chemistry at University of York for his support with the AcroSeal packaging demonstration video.

EUROPE

Austria: +43 (0)800 20 88 40

Germany: +49 2304 932-5

Finland: +358 (0)9 8027 6280

Norway: +47 22 95 59 59

Sweden: +46 31 352 32 00

Belgium: +32 (0)056 260 260

Ireland: +353 (0)1 885 5854

France: +33 (0)3 88 67 14 14

Portugal: +351 21 425 33 50

Switzerland: +41 (0)56 618 41 11

Denmark: +45 70 27 99 20

Italy: +39 02 950 59 478

Netherlands: +31 (0)20 487 70 00

Spain: +34 902 239 303

UK: +44 (0)1509 555 500

ASIA

Malaysia: +603 5122 8888 | enquiry.my@thermofisher.com **Singapore:** +65 6873 6006 | enquiry.sg@thermofisher.com

