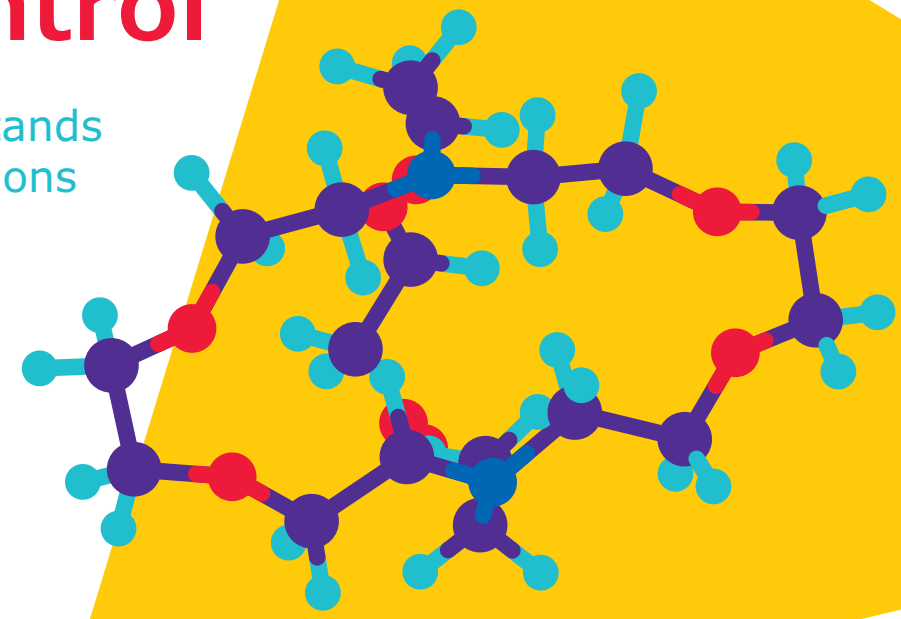
Keep Everything Under Control

Crown ethers and cryptands for demanding applications



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Lab & Production Materials

Crown ethers

Monocyclic complexing agents

Crown ethers are polyethers in which oxygen atoms are mostly connected by ethylene bridges to form a crown-like structure. Often, the ethylene bridges are also linked with one or more condensed benzene or cyclohexane rings. Alternatively, the oxygen atoms may be partially or totally substituted by heteroatoms (N, P, S) or hetero-aromatic building blocks, such as pyridine. Aromatic crown ethers may even be halogenated, nitrated or reacted with formaldehyde. Crown ethers offer the advantage of thermal stability.

Our crown ethers and cryptands offer remarkable opportunities for both synthesis and analysis. From chemical reactions involving ions, to the separation or identification of ions, you can rely on our high-quality portfolio of monocyclic and bicyclic complexing agents to solve your challenges.

Cation complexes: Coronates

Crown ethers form stable complexes with numerous cations, particularly alkali and earth alkali ions including the ammonium ion. Depending on the cation, monocyclic polyethers form 1/1 or 1/2 inclusion compounds known as coronates. In this process, the cation is locked in the cavity of the crown ether, or between two crown ether molecules. The most stable complexes are formed when the size of the crown ether cavity correlates with the diameter of the cation. The stability of the complex is also dependent on the solvent. If water is used instead of organic solvents, water molecules participate in complex formation.

- High affinity for numerous cations
- Form stable complexes (coronates) with alkali and earth alkali ions including the ammonium ion
- Stability of the complex is solvent dependent
- If present, water molecules participate in complex formation

Applications

The crown ethers' ability to bind cations in complex form while simultaneously solvatising them, enables homogeneous phase reactions to be carried out in non-polar, aprotic solvents with the participation of salts. During such a cation solvatisation, very reactive, non-solvatised ("bare") anions are liberated. Under mild conditions and in neutral media, these anions can act as strong nucleophiles, bases or oxidants. Crown ethers are also suitable for performing Wittig reactions under mild conditions.

These effects, in combination with the chemical stability of coronates and their high solubility in common solvents, demonstrate their considerable importance in chemical synthesis.

- Phase transfer catalysis
- Wittig reactions under mild conditions

Ordering information

Product	Order number	Pack size	Special ion selectivity	Diameter
Benzo-15-crown-5	8137180005	5 g	$Na^+ > K^+ > Cs^+$	1.7 – 2.2 Å
N-Phenylaza-15-crown-5	8138850005	5 g	$Na^+ > K^+ > Cs^+$	–
18-Crown-6	8116840002	2 g	$K^+ > Na^+ > Li^+$	2.6 – 3.2 Å
	8116840005	5 g		
	8116840025	25 g		
Dibenzo-18-crown-6	8117310005	5 g	$K^+ > Na^+ > Li^+$	2.6 – 3.2 Å
	8117310050	50 g		
Dicyclohexyl-18-crown-6	8118660001	1 g	$K^+ > Na^+ > Li^+$	2.6 – 3.2 Å
	8118660005	5 g		
Dibenzo-24-crown-8	8137550001	1 g	–	–
	8317550005	5 g	–	–
Kryptofix® 21	8117200001	1 g	–	–
	8117200005	5 g		
Kryptofix® 22	8109530001	1 g	–	–
	8109530005	5 g		
Kryptofix® 22 DD	8119630001	1 g	–	–

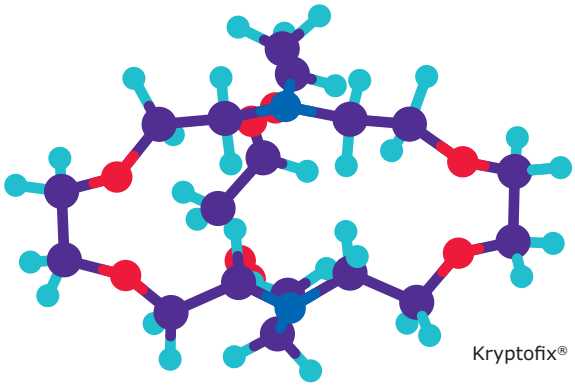
Cryptands

Bicyclic complexing agents

We produce high-quality cryptands under the trademark Kryptofix®. These compounds are azapolyethers that are related to the crown ethers. Bicyclic cryptands contain two bridgehead nitrogen atoms, which are linked by a bridge containing one or several oxygen atoms. The hollow spherical structure of these compounds allows them to form stable complexes (cryptates) with metal ions, especially alkali and earth alkali ions. Compared to crown ethers, cryptands generally offer higher cation selectivity and greater complex stability.

Cation complexes: Cryptates

The most stable complexes are multiply bridged, spherical cryptates. The stability of all cryptates depends on the solvent used, and increases substantially during transfer from water to methanol. In addition, stability decreases at lower pH values due to the protonation of bridgehead nitrogen atoms. However, high stability of the complex does not necessarily mean high selectivity. For instance, some ligands form very weak but very selective complexes.



Kryptofix® 222

Selectivity for alkali ion complexes mainly depends on the cavity size and ionic radius of the cations. For earth alkali ion complexes, high stability is contrasted with low selectivity. However, there is one type of Kryptofix®, Kryptofix® 222, with the ability to distinguish between both ions for almost all alkali / earth alkali ion pairs. Increasing ligand density leads to a preference for alkali ions over earth alkali ions. This is due to the fact that the screening effect of the complexed cation against solvent is greater for Ba^{2+} than for K^{+}. Selectivity normally increases from water to methanol, whereby complex formation with larger cations has preference over smaller ones.

- Greater selectivity and stability than crown ethers
- Form stable complexes (cryptates) with alkali and earth alkali ions
- Stability of the complex is solvent dependent
- Selectivity and stability increase from water to methanol

Applications

Thanks to their stereochemical properties, Kryptofix® compounds are highly beneficial for the separation of cation mixtures, the development of cation exchangers, the selective extraction of particular elements from salt solutions.

- Separation of cation mixtures
- Development of cation exchangers
- Reagent for synthesizing a radiotracer for the diagnostic Positron Emission Technology (PET)

Ordering information

Product	Order number	Pack size	Special ion selectivity	Diameter
Kryptofix® 221	8106468250	250 µl	$Sr^{2+} > Ca^{2+} > Ba^{2+} > Na^{+} > K^{+} > Li^{+} > Mg^{2+}$	1.15 Å
	8106460001	1 ml		
Kryptofix® 222	8106478250	250 mg	$Ba^{2+} > Sr^{2+} > K^{+} > Ca^{2+} > Na^{+} > Li^{+}, Mg^{2+}$	1.4 Å
	8106470001	1 g		
	8106470005	5 g		
Kryptofix® 222 (special quality)	8149250001	1 g	$Ba^{2+} > Sr^{2+} > K^{+} > Ca^{2+} > Na^{+} > Li^{+}, Mg^{2+}$	1.4 Å

Related Compounds

Product	Order number	Pack size	Special ion selectivity	Diameter
Kryptofix® 5	8116890005	5 g	–	–

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