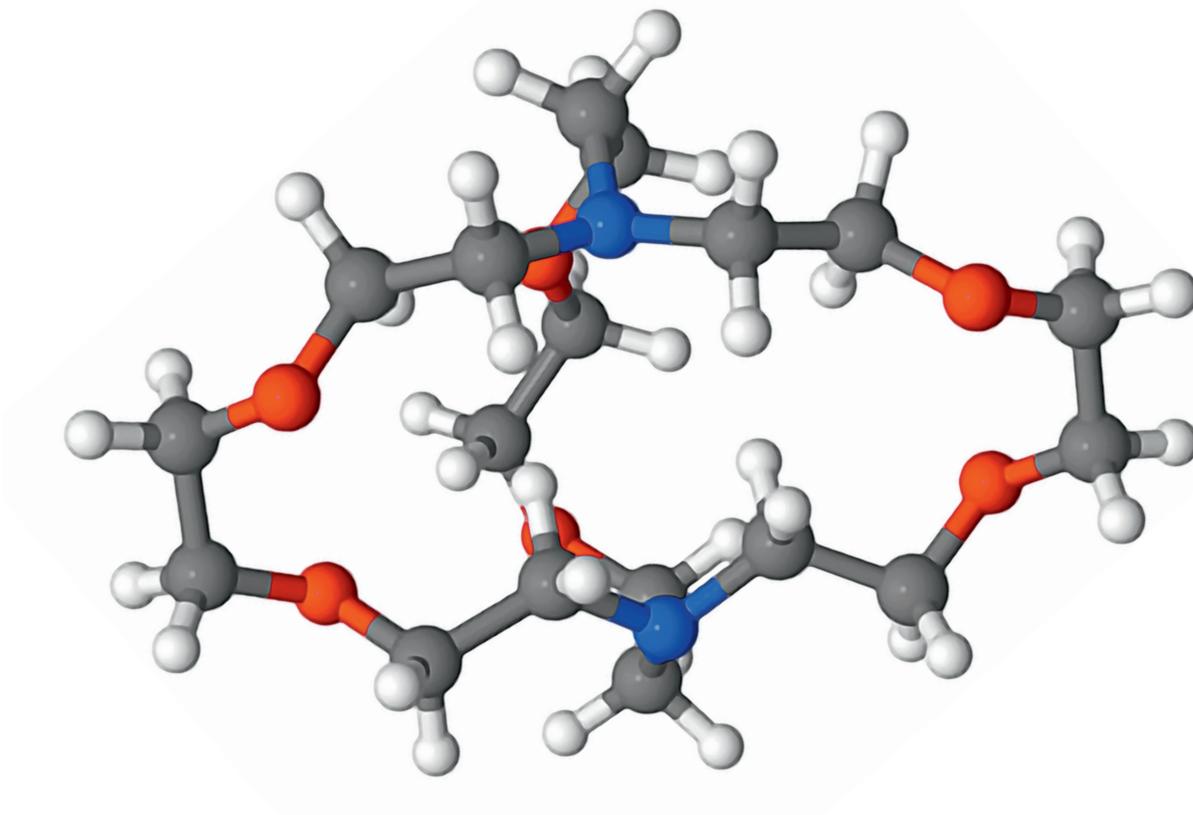


Keep everything under control Crown ethers and Kryptofix[®] for professional applications

EMD Millipore's crown ethers and Kryptofix[®] compounds 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 macrobicyclic complexing agents to solve your challenges.



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 oxygen atoms 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.

Cation complexes: Coronates

Crown ethers form stable complexes with numerous cations, particularly alkali and alkaline earth ions including the ammonium ion. Depending on the cation, macrocyclic 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.

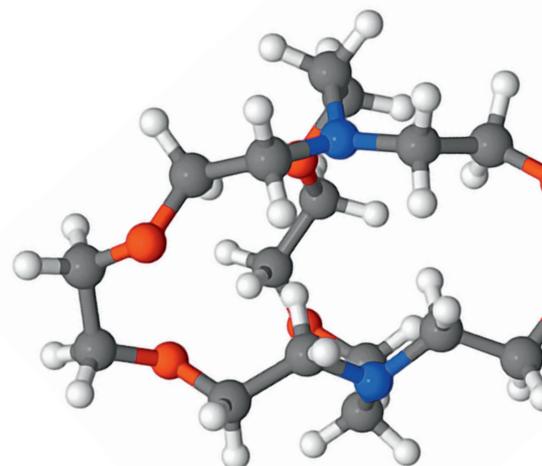
- High affinity for numerous cations
- Form stable complexes (coronates) with alkali and alkaline earth ions including the ammonium ion
- Stability of the complex is solvent dependent
- If present, water molecules participate in complex formation

Applications

The crown ethers' ability to bind cations in complex form while simultaneously solvating them, enables homogenous phase reactions to be carried out in non-polar, aprotic solvents with the participation of salts. During such a cation solvation, very reactive, non-solvated ("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	VWR Cat. No.	Pack size	Special ion selectivity	Diameter
12-Crown-4	EM8.13714.0006	5 ml	Li ⁺	1.2 – 1.5 Å
15-Crown-5	EM8.13715.0006	5 ml	Na ⁺ > K ⁺	1.7 – 2.2 Å
	EM8.13715.0025	25 ml		
Benzo-15-crown-5	EM8.13718.0005	5 g	Na ⁺ > K ⁺ > Cs ⁺	1.7 – 2.2 Å
N-Phenylaza-15-crown-5	EM8.13885.0005	5 g	Na ⁺ > K ⁺ > Cs ⁺	–
18-Crown-6	EM8.11684.0002	2 g	K ⁺ > Na ⁺ > Li ⁺	2.6 – 3.2 Å
	EM8.11684.0005	5 g		
	EM8.11684.0025	25 g		
Benzo-18-crown-6	EM8.14316.0001	1 g	K ⁺ > Cs ⁺ > Na ⁺	2.6 – 3.2 Å
Decyl-18-crown-6	EM8.24438.0500	500 mg	K ⁺ > Na ⁺ > Li ⁺	~2.9 Å
Dibenzo-18-crown-6	EM8.11731.0005	5 g	K ⁺ > Na ⁺ > Li ⁺	2.6 – 3.2 Å
	EM8.11731.0050	50 g		
Dicyclohexyl-18-crown-6	EM8.11866.0001	1 g	K ⁺ > Na ⁺ > Li ⁺	2.6 – 3.2 Å
	EM8.11866.0005	5 g		
Dibenzo-24-crown-8	EM8.13755.0001	1 g	–	–
	EM8.13755.0005	5 g	–	–

Kryptofix® compounds

Macrobicyclic neutral ligands

EMD Millipore produces high-quality cryptands under the trademark Kryptofix®. These compounds are azapolyethers that are related to the crown ethers. Polycyclic 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 alkaline earth 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.

Selectivity for alkali ion complexes mainly depends on the cavity size and ionic radius of the cations. For alkaline earth ion complexes, high stability is contrasted with low selectivity. However, there is one type of Kryptofix® e.g. Kryptofix® 222, with the ability to distinguish between both ions for almost all alkali / alkaline earth ion pairs. Increasing

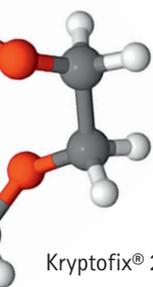
ligand density leads to a preference for alkali ions over alkaline earth ions. This is due to the fact that the screening effect of the complexed cation against solvent is greater for Ba²⁺ than for K⁺. Selectivity normally increases from water to methanol, whereby complex formation with larger cations has preference over smaller ones.

- Greater selectivity and stability than crown ethers
- Form stable complexes (cryptates) with alkali and alkaline earth 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 or for body detoxification (e.g. the decorporation of traces of heavy metals).

- Separation of cation mixtures
- Development of cation exchangers
- Selective extraction of ions from salt solutions or for body detoxification



Kryptofix® 222

Ordering information

Product	VWR Cat. No.	Pack size	Special ion selectivity	Diameter
Kryptofix® 5	EM8.11689.0005	5 g	-	-
Kryptofix® 21	EM8.11720.0001	1 g	-	-
	EM8.11720.0005	5 g		
Kryptofix® 22	EM8.10953.0001	1 g	-	-
	EM8.10953.0005	5 g		
Kryptofix® 221	EM8.10646.0050	250 µl	Sr ²⁺ > Ca ²⁺ > Ba ²⁺ > Na ⁺ > K ⁺ > Li ⁺ > Mg ²⁺	1.15 Å
	EM8.10646.0001	1 ml		
Kryptofix® 222	EM8.10647.8250	250 mg	Ba ²⁺ > Sr ²⁺ > K ⁺ > Ca ²⁺ > Na ⁺ > Li ⁺ , Mg ²⁺	1.4 Å
	EM8.10647.0001	1 g		
	EM8.10647.0005	5 g		
Kryptofix® 222 (special quality)	EM8.14925.0001	1 g	Ba ²⁺ > Sr ²⁺ > K ⁺ > Ca ²⁺ > Na ⁺ > Li ⁺ , Mg ²⁺	1.4 Å

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