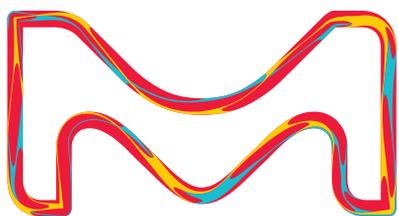
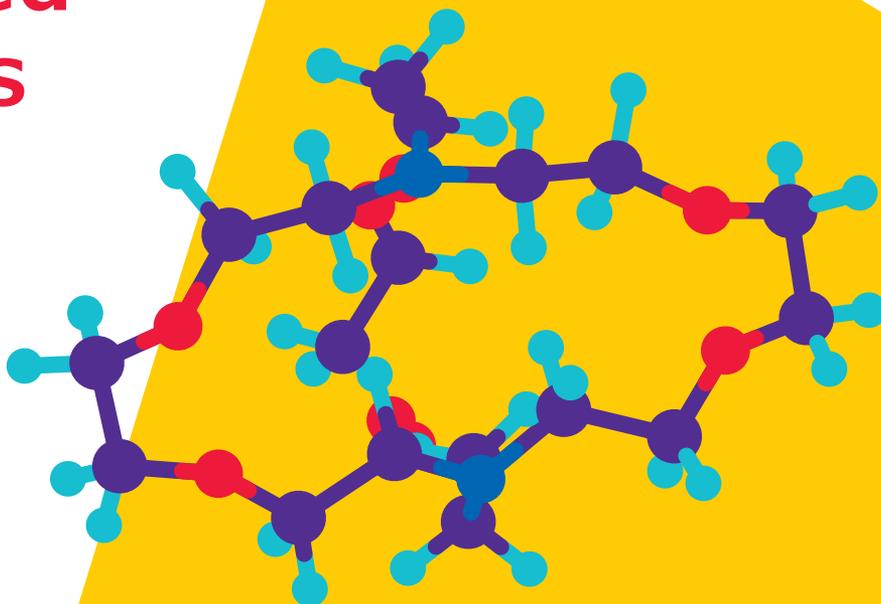


Crown ethers and cryptands for advanced applications



The life science
business of Merck
operates as
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Sigma-Aldrich[®]
Lab & Production Materials

Crown ethers

Monocyclic complexing agents

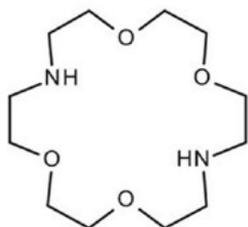
Crown ethers are polyethers in which oxygen atoms are mostly connected by ethylene bridges to form a crown-like structure. Often, the ethylene bridges are also linked with one or more condensed benzene or cyclohexane rings. Alternatively, the oxygen atoms may be partially or totally substituted by heteroatoms (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.

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.

Ordering information

| Product | Order number | Pack size | Special ion selectivity | Diameter |
|-------------------------|--------------|-----------|--|-------------|
| 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® 22 | 8109530001 | 1 g | - | - |
| | 8109530005 | 5 g | - | - |



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.

Applications

The crown ethers' ability to bind cations in complex form while simultaneously solvating them, enables homogeneous 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.

Cryptands

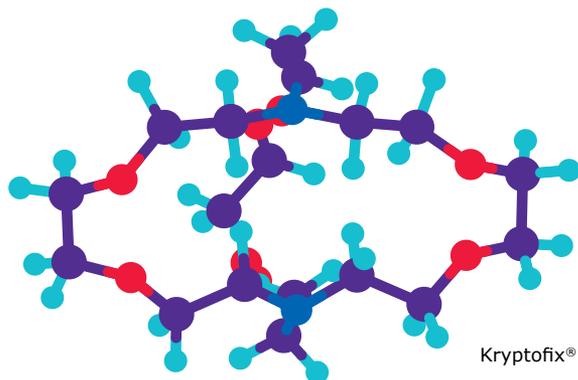
Bicyclic complexing agents

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.

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 Ba²⁺ than for K⁺. Selectivity normally increases from water to methanol, whereby complex formation with larger cations has preference over smaller ones.



Kryptofix® 222

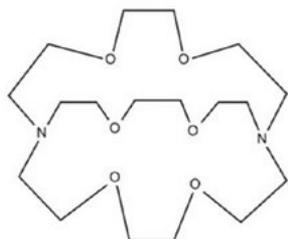
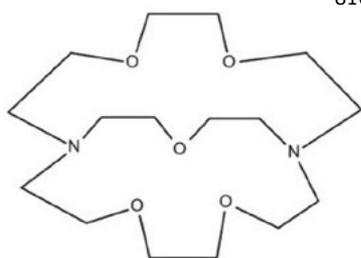
Applications

Thanks to their stereochemical properties, Kryptofix compounds have highly beneficial uses including:

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

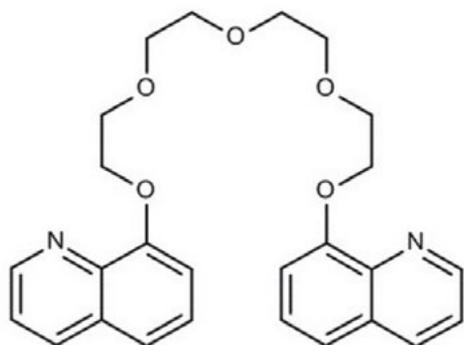
Ordering information

| 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 | - | - |



To place an order or receive technical assistance in Europe, please call Customer Service:

France: 0825 045 645

Spain: 901 516 645 Option

Germany: 069 86798021

Switzerland: 0848 645 645

Italy: 848 845 645

United Kingdom: 0870 900 4645

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Or visit: [SigmaAldrich.com/Offices](https://www.SigmaAldrich.com/Offices)

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