

## JBS Tantalum Cluster Derivatization Kit

Cat. No.	Amount
PK-103	6 mg

For *in vitro* use only

Quality guaranteed for 12 months

Store at room temperature under an argon atmosphere. Once the vials have been opened floating with argon is recommended for long term storage.

### Application

Heavy atom derivatization of biological macromolecules for isomorphous and/or anomalous phasing methods.

### Kit Contents

6 pre-weighted solid aliquots of hexatantalum tetradecabromide at 1 mg.

### Specifications

Name: Hexatantalum tetradecabromide

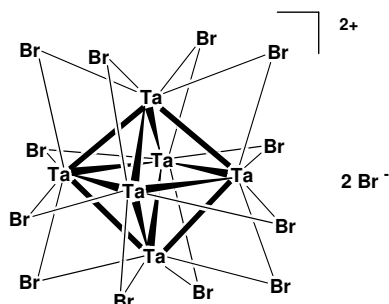
Formula:  $[\text{Ta}_6\text{Br}_{12}]^{2+} \times 2 \text{Br}^-$

MW: 2204,3 g/mol

Appearance: green powder

Water Solubility: ~ 2 mM

Manufacturer:  proteros  
 biostructures



### Features

The Tantalum Bromide Cluster is used for the preparation of heavy-atom derivatives for structure determination of biological macromolecules by X-ray analysis. Electron-rich compounds are utilized in single and multiple isomorphous replacement (SIR and MIR)

in order to induce measurable changes of the diffraction intensities required for phase calculation.

Furthermore, the Tantalum Bromide Cluster contains two strong anomalous scatterers suitable for multiple anomalous diffraction (MAD) experiments:

Ta L-III 9.8811 keV (1.2548 Å)

Br K 13.4737 keV (0.9202 Å)

The hexatantalum bromide cluster is built of an octahedron of 6 metal atoms with 12 bridging bromine atoms along the 12 edges of the octahedron. The cluster is highly symmetrical and has a radius of approximately 4.3 Å.

Tantalum Bromide Clusters have been successfully employed in several structural studies because of their high electron-density, solubility in aqueous solutions and stability over a wide pH range [1-4].

### Usage

Heavy-atom derivatization is performed by either:

- Adding solid Tantalum Bromide Cluster directly to the crystallization drop:
  - Grasp a few crumbs of the solid Tantalum Bromide Cluster with a micro-spatula and add them to the crystallization drop containing pre-grown protein crystals. The metal cluster will dissolve within a few hours and the protein crystals will turn green.

or

- Transferring the crystal from the drop into a soak solution containing the **Tantalum Bromide Cluster**:
  - Soaking needs to be performed in a stabilizing solution, wherein the protein crystal is stable. The composition of the stabilizing solution has to be determined experimentally. Since the crystallization drop contains saturated solution of protein molecules, the stabilization solution usually has a somewhat higher concentration of precipitant or buffer than the crystallization drop.

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- Add 230  $\mu$ l stabilizing solution to a solid aliquot to yield a soak solution containing 2 mM Tantalum Bromide Cluster. Add more if you require a more diluted solution.
- Fill the reservoir well of a sitting drop plate with the stabilizing solution (without the metal cluster) and the protein well with the freshly prepared soak solution containing the Tantalum Bromide Cluster.
- Transfer a crystal from the crystallization drop into the soak solution using a loop, a MicroMount™ or a MicroMesh™.

### Soaking Time

The soaking time depends on a number of variables such as the concentration of the cluster, temperature, composition of the soaking solution and the protein under investigation.

The soaking time can vary from 1 hour to several weeks. For initial screening for binding we recommend one hour up to one day. If the protein crystals turn green soaking is usually sufficient and diffraction of the crystals can be tested.

### Phasing

At low resolution ( $< 6 \text{ \AA}$ ) it can be assumed that all atoms of the cluster scatter in phase. Therefore, the cluster can be considered as a "super heavy atom", easily to locate in the isomorphous difference Patterson map. At high resolution the individual atoms of the cluster can be used for phasing after positioning the cluster in the unit cell [1].

### Safety Information

Heavy atom compounds are toxic substances and should be treated as such.

Work carefully and clean when handling heavy atom compounds.

Wear gloves when handling heavy atom reagents. Wear gloves when handling crystals and any laboratory material that was in contact with heavy atom compounds.

Keep in mind that all glassware and laboratory material (such as spatulas etc.) that have been in contact with heavy atom compounds must be considered as contaminated and should be handled accordingly.

Label all plates and lab ware containing heavy atom compounds appropriately.

Get to know the appropriate hazardous material guidelines for handling and disposal of heavy atom compounds, heavy atom reagents, and laboratory equipment contaminated with heavy atoms.

### References

- [1] Knäblein *et al.* (1997)  $\text{Ta}_6\text{Br}_{12}^{2+}$ , a tool for phase determination of large biological assemblies by X-ray crystallography. *J. Mol. Biol.* **270**:1.
- [2] Yonath *et al.* (1998) Crystallographic studies on the ribosome, a large macromolecular assembly exhibiting severe nonisomorphism, extreme beam sensitivity and no internal symmetry. *Acta Cryst.* **A54**:945.
- [3] Gomis-Rüth *et al.* (2001) Solving a 300 kDa multimeric protein by low-resolution MAD phasing and averaging/phase extension. *Acta Cryst.* **D57**:800.
- [4] Szczepanowski *et al.* (2005) Crystal structure of a fragment of mouse ubiquitin-activating enzyme. *J. Biol. Chem.* **280**:22006.