Heavy Atom Screens™

HAMPTON RESEARCH
Solutions for Crystal Growth

User Guide

Introduction

Multiple isomorphous replacement is the predominant method for determining the initial phasing of completely new biological macromolecular structures. The approach requires at least one and in many cases numerous heavy atom derivatives of the macromolecule. The search for isomorphous derivatives is sometimes as empirical as determining preliminary crystallization conditions. Numerous heavy atoms must typically be screened before one or more is found that binds without damaging the crystal or disrupting the crystal lattice.

The Hampton Research Heavy Atom Screens are designed to offer convenient sets of "popular" heavy atom compounds. The sets are based upon those heavy atom compounds with regard to their frequency of use in MIR and SIR structure solution from published crystallographic structures.

Hampton Research Heavy Atom Screening Kits:

HR2-442 Heavy Atom Screen Pt	HR2-448 Heavy Atom Screen M1
HR2-444 Heavy Atom Screen Au	HR2-450 Heavy Atom Screen M2
HR2-446 Heavy Atom Screen Hg	

Warning

Treat all heavy atoms reagents as toxins. Refer to the enclosed Material Safety Data Sheets for safety information.

Familiarize yourself with the appropriate safety procedures for handling heavy atom reagents. It is highly recommended that one consult the literature and the advice of experienced crystallographers before beginning heavy atom work.

Do not rush through a heavy atom experiment.

Wear gloves when handling heavy atom reagents. Wear gloves when handling crystals, plates, capillaries, and cryo materials that involved heavy atom reagents.

Remember to remove gloves used to handle heavy atoms before touching anything else (doorknobs, telephones, yourself, etc...).

Volatile reagents containing heavy atoms, especially mercury should be handled in a fume hood.

Although some heavy atoms can be removed from glassware using a nitric acid wash, keep in mind that all glassware, spatulas, and labware coming into contact with any heavy atom is considered contaminated.

Label all plates, capillaries, and cryo labware containing heavy atoms appropriately.

When weighing heavy atom reagents it is recommended to do so directly into small polyethylene vials used to generate working stocks rather than onto weigh paper and risk transfer errors.

Check with your department's hazardous material guidelines for proper handling and disposal of heavy atoms, heavy atom reagents, and labware contaminated with heavy atoms.

Uranium and thorium compounds are radioactive and are not included in the Hampton Research Heavy Atom Screens. Just the same, follow radiation safety rules in addition to the usual safety rules when working with uranium and thorium compounds.

Preparation of Heavy Atom Solutions

Many heavy atom compounds are unstable in solution, hence freshly prepared soaking solutions should be prepared whenever possible.

Screening for Heavy Atom Derivatives

It is often the case that many (25 to 75) heavy atoms need to be evaluated before a successful isomorphous derivative is found. Screening and patience is an essential part of heavy atom derivatization.

Which Heavy Atom To Try?

One must be sure to choose heavy atoms that ensure the difference in diffraction amplitudes owing to the heavy atom are larger than the errors in data collection. The atomic number of the heavy atom and the number of derivatized sites required for successful phasing are proportional to the molecular weight of the macromolecule. Larger macromolecules may require heavy atoms of higher atomic number and more than one heavy atom per molecule.

Amino Acid Composition Tips

No free cysteines or histidines?

- Try non-mercurials.

Normal distribution of amino acids?

- Try platinum which binds mainly methionine, histidine, and cysteine residues.

Positively charged residues?

- Try $Pt(CN)_2$.

Free cysteine and histidine?

- Try mercurials.

For a discussion of the reactivities of amino acids see "Favorite 5 (IV)."

Favorite Five (IV)

1. K_2PtCl_4 at pH 6.0 or higher in ammonia free media.
2. Ethylmercury phosphate in phosphate free media, pH 6.0 or higher.
3. Samarium acetate or uranyl acetate in phosphate free media.
4. K_2HgI_4 with excess KI.
5. $K_2Pt(CN)_4$.

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All the above heavy atoms, except for uranyl acetate can be found in the Hampton Research Heavy Atom Screen series.

Procedure

Heavy atom derivatization is typically performed by either adding a heavy atom solution to the drops (mother liquor) containing the crystal(s) or transferring the crystal(s) from the mother liquor drop to a stabilizing solution containing the heavy atom. Note: the mother liquor is the solution from which the crystals was grown and contains a saturated solution of macromolecule, the macromolecular crystal, and the crystallization reagents. The stabilizing solution does not contain the saturated macromolecular solution or a crystal but will contain the crystallization reagent with adjustments made to compensate for the lack of the saturated macromolecular solution. One must empirically determine what adjustments must be made to the mother liquor to create a stabilizing solution where the heavy atom and macromolecular crystal can be added without damaging the crystal. Typically, the stabilizing solution will have a slightly higher concentration of precipitant or buffer than the mother liquor. Crystals grown from low salt can sometimes be stabilized with the addition of PEG or MPD.

Preparing the Heavy Atom Soak Solution

Just prior to derivatization experiments prepare a fresh solution of the heavy atom in the stabilizing solution. Try a 1 to 10 mM heavy atom concentration in the stabilizing solution using polypropylene microcentrifuge tubes. This is the *Heavy Atom Soak Solution*. Typical concentrations of heavy atom range of 1 mM to 100 mM depending upon the pH, temperature, crystallization reagent, and heavy atom.

Applying the Heavy Atom Soak Solution

Prepare a crystallization plate for a hanging drop vapor diffusion experiment. The reservoir(s) should contain the stabilizing solution minus the heavy atom. Pipet 2 to 10 microliters of Heavy Atom Soak Solution onto a siliconized cover slide. During the initial period of heavy atom screening one should use the smallest crystals, saving the best crystals for once a successful Heavy Atom Soak Solution has been determined.

Transfer a crystal from the mother liquor to the Heavy Atom Soak Solution drop using a Mounted CryoLoop, Tungsten Wire, Pipet, or Capillary. Try to minimize the amount of mother liquor transferred with the crystal as this will dilute the Stabilizing Solution.

Allow the crystal(s) to soak overnight.

Observing the Results

Observe the crystal(s) under a light microscope (10 to 100x magnification) for cracks, visible degradation, loss of birefringence, or dissolution. Those crystals that appear to have been damaged during the initial soak experiment should be tested for X-ray diffraction to assure the crystal is damaged. If the crystal is damaged, the concentration of heavy atom in the Heavy Atom Soak Solution should be diluted two to five fold and additional soak experiments be performed until crystals survive the initial soaking stage. Crystals that are visibly satisfactory but diffract to low resolution or demonstrate a substantial increase in mosaicity should also be tested in a diluted Heavy Atom Soak Solution.

It is possible that crystals will not survive this initial stage for certain heavy atoms. This is why multiple heavy atom reagents should be screened during the initial stage of heavy atom derivatization. Once a crystal from a Heavy Atom Soak Solution demonstrates diffraction, one should collect a few frames of consecutive degrees of oscillation data in an orientation that maximizes redundancy. Increase exposure times if necessary to compensate for smaller crystal volume. If significant intensity differences exist between the native crystal X-ray data and the crystals from the heavy atom soaks, transfer a good crystal to the Heavy Atom Soak Solution to be used for collection of a full derivatized data set. The use of cryocrystallographic methods can make it possible to collect full data sets from a single derivatized crystal, but to be safe, to increase the probability of getting the same degree of occupancy and allowing the merging of data from multiple crystals into one data set use the same Heavy Atom Soak Solution when derivatizing multiple crystals.

General Observations About Heavy Atoms

$Pt(NH_3)_2Cl_2$ can be formed in about 24 hours by placing $PtCl_4$ in Ammonium sulfate above pH 7.

HgI_3 can be formed from K_2HgI_4 with the addition of excess KI.

Lanthanides appear to be more selective than uranyl ions.

Uranyl compounds often give multisite substitution.

Samarium and lead often give one major site.

Soaking

Soaking macromolecular crystals in a solution containing heavy atoms have been reported in the literature far more than co-crystallization with the heavy atoms. The solvent channels in macromolecular crystals allow heavy atom reagents to diffuse into and through the crystals and provide access to the protein in the crystal lattice. Heavy atom binding sites are accessible from adjacent protein molecules in the crystal lattice.

Soaking Time

The soaking time for heavy atom binding depends upon a number of variables such as the heavy atom, concentration of the heavy atom, solubility of the heavy atom, temperature, and the crystallization reagent. Soaking time can vary from several hours to months. For initial screening for binding, one to two days is typically sufficient.

If after soaking, the crystal appearance is unchanged from the native crystal and no changes are observed in the diffraction pattern then one might try increasing the soaking time and the concentration of the heavy atom. If after soaking, the crystal cracks or the diffraction pattern changes too much, or the diffraction resolution dramatically decrease then one should screen lower concentrations of the heavy atom and evaluate shorter soak times.

Concentration of Heavy Atoms

Typically 1 mM should be the starting value of the concentration of the heavy atom in the presence of the mother liquor and crystal. Therefore, a small stock solution (make no more than is essential!) of 10 mM is an appropriate working stock which can be diluted into the mother liquor containing the crystal.

Concentrations of heavy atoms as low as 0.05 mM and as high as 100 mM have been reported.

Increasing the concentration of the heavy atom can decrease soak times and sometimes give rise to specific binding at a further site (7).

Many heavy atoms are only sparingly soluble in water. Addition of these reagents to macromolecular crystals can be accomplished by solubilizing the heavy atom in a carrier solvent that is less polar than water. Acetonitrile is a frequently used carrier solvent. Dissolve the heavy atom in the carrier solvent and then pipet the carrier solvent with heavy atom into the crystal mother liquor such that the final carrier solvent concentration in the crystal mother liquor is 3 to 5% v/v. Volatile reagents containing heavy atoms should be handled in a fume hood.

Derivatize Then Crystallize?

In some cases one can first derivatize the protein with the heavy atom then attempt crystallization. This procedure is less frequently used since the procedure may not produce derivatized crystals which are isomorphous with the native crystals because the positioning of the heavy atom may disrupt intermolecular contacts. Sometimes the presence of the heavy atom with the native macromolecule in solution can change the solubility of the macromolecule which in turn can change the crystallization conditions. The native and derivatized now crystallize under different conditions and thus one must screen for new crystallization conditions. Also, with the macromolecule free in solution it is possible that additional heavy atom sites are now introduced (which can complicate phasing) since sites previously hidden by crystal contacts are now exposed. However, the method can be useful when one is trying to derivatize the macromolecule with a heavy atom or heavy atom - ligand complex that is too large to diffuse into and through the crystal's solvent channels.

Derivation by Dialysis

Rather than place the crystal directly into the soaking solution, or placing the heavy atom reagent directly into the mother liquor containing the crystal, one may dialyse the crystal in mother liquor versus the heavy atom in mother liquor (5, 6).

Metal Ion Replacement

With macromolecules that bind a metal ion cofactor (zinc, calcium, cadmium), the metal ion can be removed and replaced by a heavy atom to provide an isomorphous derivative. One may place the crystal containing the metal ion cofactor into mother liquor containing the heavy atom and hope for exchange. One may crystallize the macromolecule without the metal ion cofactor but must be careful of non-crystallization or non-isomorphous crystals. One may crystallize the macromolecule in the presence of the metal ion cofactor, then soaking the crystals in a suitable chelating agent (EDTA, EGTA, or Chelating Resin - Hampton Research Catalog Number: HR2-312).

Crystallization Reagents and Heavy Atoms

Crystallization reagents (specifically salts) and buffers are a potential ligand source for heavy atoms. The heavy atom may complex with the salt which can precipitate the heavy atom and/or crystallization reagents and interfere with the reaction of the heavy atom with the protein. Heavy atom reagents are typically less soluble in high salt. Hence high salt concentrations are not the ideal medium for heavy atom reactions with macromolecules.

Polyethylene glycol does not react with most heavy atom compounds and is a favorable media for heavy atom reactions.

Above pH 6 ammonium sulfate (ammonium ion can dissociate at higher pH) is a poor reagent for heavy atom binding because of the presence of the nucleophile NH3 (1). If possible, crystals should be transferred to magnesium, lithium, or sodium sulfate, sodium phosphate, potassium phosphate, or even polyethylene glycol.

Tris, phosphate, citrate, beta-mercaptoethanol, and dithiothreitol have been reported to interfere with heavy atom binding in some instances.

Excess phosphate is undesirable for uranium and rare earth metals.

Excess phosphate can displace chloride from K_2PtCl_4.

Acetate can complex uranyl and lanthanide ions and decrease their reactivity.

Citrate can complex uranyl and lanthanide ions and decrease their reactivity worse than acetate.

Uranyl and lanthanide ions form insoluble phosphates and hydroxides.

Platinum and mercury do better in phosphates than sulfates.

The formation of platinum phosphate complexes can be minimized by a large excess of acetate and no chloride.

Platinum, mercury, and gold tend to bind to sulfhydryl, imidazole, and thiothers rather than carboxylate or hydroxyl groups.

Avoid phosphate buffers when using ethyl mercury phosphate.

Physical Influences on Heavy Atoms

pH and Heavy Atoms

The preparation of isomorphous heavy atom derivative crystals will depend upon the pH of the solution. The most successful pH range for heavy atom soaking is 6 to 8. When the pH is below 6, reactive groups on the macromolecule which could bind the metal are protonated (such as glutamic and aspartic acid) and blocked. Since the pH of the mother liquor will determine the protonation state of amino acid residues in the protein chain it is worthwhile to try several different pH values when screening for heavy atoms. Many heavy atom compounds are alkaline labile and form insoluble hydroxides at high pH. Refer to pages 6-10 for specific pH attributes of some heavy atoms.

Temperature and Heavy Atoms

The temperature can change the rate of heavy atom binding and the degree of binding. In most cases, the heavy atom binding temperature is the same as the crystallization temperature. Typically, lower temperature result in slower reaction rates and elevated temperature result in higher reaction rates (8).

Photosensitivity

Many heavy atom compounds are light sensitive. Therefore, following the set up, soakings should be performed in low illumination or in the dark. A cupboard, drawer, incubator or box is generally sufficient in providing low light levels.

Disorder

The introduction of heavy atoms into the native crystals can introduce disorder. Significantly larger temperature factors of the derivative data compared to the native data is a sign of disorder. Sometimes back-soaking can reduce such crystal changes. For back-soaking, the crystals are transferred from the original soak solution to a solution with a lower concentration of heavy atom (for example, from 1 mM to 0.1 mM), or even to the original mother liquor without heavy atom. This procedure can reduce heavy atom binding to only the lower affinity sites. If back-soaking is unsuccessful one should try preparing new heavy atom derivatives in lower concentrations of heavy atom.

Cross-Linking Crystals

Cross-linked crystals can be more resilient to reagent changes in the mother liquor. Cross-linked crystals often retain constant cell dimensions, as well as activity and structure. Soaking the crystals in 0.01% to 3% glutaraldehyde for a period of minutes to hours is often sufficient for successful cross-linking. Therefore, if heavy atom binding causes crystal damage even at low heavy atom concentrations, prior cross-linking may prevent damage from occurring.

Selective cross-linking has been performed using bifunctional diimidates which cross-link between the epsilon amino groups of lysine residues. Reagents such as dimethyl malonic diimidate, dimethyl dodecanoic diimidate at concentrations of 2 mg/ml have been successfully used to cross-link macromolecular crystals (2, 3). One might also consider adipaldehyde.

Crosslinking crystals might also be useful in stabilizing macromolecular crystals when derivatizing crystals which were grown in low ionic strength media (via dialysis or vapor diffusion in low ionic strength, i.e. PEG) where the introduction of a heavy atom can increase the ionic strength of the mother liquor.

Classification of Heavy Atoms

Much of the literature separates heavy atom reagents into two classes: Class A and Class B metals (d).

Class A

Class A metals have a preference for hard ligands such a carboxylates and other oxygen containing groups. The Class A metals consist of the alkali metals (Li, Na, K, Rb, Cs), the alkaline earth metals (Mg, Ca, Sr, Ba) the lanthanides (La, Ce, Nd, Sm, Eu, Gd, Dy, Er, Lu), and the actinide (UO_2). Tl and Pb have a mixed Class A and B character and can coordinate similar to true Class A metals. Class A metals do not polarize well and bind electronegative, hard ligands such as F, OH, H_2O, phosphate, and carboxylates in an electrostatic fashion. Interactions between the macromolecule and Class A metals are weakened in high ionic strength reagents and mother liquors. Class A metals can form insoluble hydroxides at alkaline pH levels (>7.5). Phosphates and citrates compete for Class A Metals in solution. Class A metals can be used at low pH. Class A metals do not compete with NH_3. Class A metals can substitute for Na, K, Mg, or Ca. Examples of Class A metals include Uranium, Lanthanide, Thallium, and Lead.

Class B

Class B metals have a preference for soft ligands such as sulfur, nitrogen and halides. The Class B metals are polarizable. They do not work well at low pH since many of their ligands such as histidine and cysteine are protonated at low pH and thus less reactive. However, Pt is an exception since Pt can interact with methionine and disulphide bridges at low pH. In the presence of ammonium sulfate and pH above 7 the Class B metals do not function well since NH_3 will compete for the heavy atom. Phosphates and hydroxides are less of a problem with Class B metals since they are hard ligands and

do not bind tightly to Class B metals. Class B metal and macromolecule interactions are less sensitive to high ionic strength than Class A metal and macromolecule interactions. Class B metals can form stable heavy atom complexes with macromolecules through anionic, cationic, or hydrophobic interactions in conditions where Class B metals do not typically function well. Examples of Class B metals include Mercury, Silver, Platinum, Gold, Palladium, Iridium, Osmium, and Cadmium.

Other classifications of heavy atom reagents include Anionic, Cationic, Hydrophobic, and Other (d).

Anionic

Anionic heavy atom reagents predominantly interact with the macromolecule through their overall negative charge and are typically less effective at high ionic strength and in the presence of other anions which may compete for a similar site. Binding is typically enhanced at lower pH where the macromolecule will be more positively charged. Examples include I, HgI_3, $Pt(CN_4)_2$, $IrCl_6$, and $Au(CN)_2$.

Cationic

Cationic heavy atom reagents predominantly interact with the macromolecule through their overall positive charge and are typically less effective at high ionic strength and in the presence of other cations which may compete for a similar site. Binding is typically enhanced at higher pH where the macromolecule will be more negatively charged. Examples include NH_3 and its potential derivatives such as $Pt(NH_3)_4$, $Ir(NH_3)_6$, $Hg(NH_3)_2$, and $Au(NH_3)_4$.

Hydrophobic

Hydrophobic heavy atom reagents predominantly interact with macromolecules by penetrating the hydrophobic interior. Xenon is an example of a hydrophobic heavy atom reagent. Xenon derivatives are typically created by pressurizing the macromolecular crystal under xenon gas, freezing the crystal, and then collecting data at cryogenic temperatures. Other compounds with hydrophobic tendencies include ethyl mercury chloride, ethyl mercury phosphate (no phosphates please!), $Pt(NH_3)_2Cl_2$, HgI_3, and Iodine (although anionic, iodine can enter proteins).

Other

Other heavy atom reagents include:

- Iodine when it is used to create mono- or di- iodinate tyrosine residues.
- Selenium which is typically incorporated into proteins as selenomethionine for MAD phasing techniques.

Amino Acid Reactivity with Heavy Atoms

Sometimes the choice of heavy atoms, the appropriate pH, and mother liquor composition can be made from examining the amino acid composition of the macromolecule. The following reference is recommended for learning more about the specific reactivities of amino acids with heavy atoms:

Petsko, G.A., Preparation of Isomorphous Heavy-Atom Derivatives, in Wyckoff, H.W., Hirs, C.H.W. and Timasheff, S.N. ed. (1985). Methods in Enzymology, Vol. 114. Diffraction Methods for Biological Macromolecules Part A. Academic Press, Orlando, pp. 147-156.

References and General Reading

References for Heavy Atom Derivatization

1. P. Sigler and D. Blow (1965). J. Mol. Biol., 14, 640.
2. V. Dombraadi et al (1980). Biochemistry, 19, 2295.
3. A. Lorek et al (1984). Biochem. J., 218, 45.
4. E. Stura and P. Chen (1992). Crystallization of Nucleic Acids and Proteins, A Practical Approach, edited by A. Ducruix and R. Giege. 241-254. Oxford University Press.
5. B. Tilander, B. Strandberg and K. Friborg (1965) J. Molec. Biol., 12, 740.
6. W. Lipscomb et al (1966). J. Molec. Biol., 19, 423.
7. M. Adams (1969). Nature, 224, 491.
8. F. Salemme et al (1973). J. Biol. Chem., 248, 3910.

General Reading for Heavy Atom Experimentation

1. Crystallographic Methods and Protocols (1996). Edited by C. Jones, B. Mulloy and M. Sanderson. Humana Press.
2. Protein Crystallography (1976). T. Blundell and L. Johnson. Academic Press.
3. Methods in Enzymology, Volume 276, Macromolecular Crystallography, Part A (1997). Edited by C. Carter and R. Sweet. Academic Press.
4. Petsko, G.A., Preparation of Isomorphous Heavy-Atom Derivatives, in Wyckoff, H.W., Hirs, C.H.W. and Timasheff, S.N. ed. (1985). Methods in Enzymology, Vol. 114. Diffraction Methods for Biological Macromolecules Part A. Academic Press, Orlando, pp. 147-156.

Internet Resources for Heavy Atom Derivatization

1. http://www.bmm.icnet.uk/had/index.html
(HEAVY-ATOM DATABANK, Suhail A. Islam, David Carvin, Michael J.E. Sternberg & Tom L. Blundell)
2. http://www.hamptonresearch.com/hrproducts/hascreens.html
(Hampton Research Heavy Atom Kits)
3. http://www.hamptonresearch.com/support/links.html
(Hampton Research Helpful Links)

Technical Support

Inquiries regarding Heavy Atom reagent formulation, interpretation of screen results, optimization strategies and general inquiries regarding crystallization are welcome. Please e-mail, fax, or telephone your request to Hampton Research. Fax and e-mail Technical Support are available 24 hours a day. Telephone technical support is available 8:00 a.m. to 5:00 p.m. USA Pacific Standard Time.

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Heavy Atom Screen Pt - Catalog Number: HR2-442

Name	Synonym	Formula	MW	pH Min	pH Mean	pH Max
1. Potassium tetrachloroplatinate(II)	1. n/a	1. K_2PtCl_4	1. 415.11	1. 3.0	1. 6.5	1. 9.1
2. Ammonium tetrachloroplatinate(II)	2. n/a	2. $(NH_4)_2PtCl_4$	2. 372.98	2. 7.5	2. 7.5	2. 7.5
3. Potassium hexachloroplatinate(IV)	3. n/a	3. K_2PtCl_6	3. 486.01	3. 4.2	3. 6.2	3. 8.4
4. Potassium tetranitroplatinate(II)	4. n/a	4. $K_2Pt(NO_2)_4$	4. 457.32	4. 2.0	4. 6.6	4. 8.6
5. Potassium tetracyanoplatinate(II) hydrate	5. n/a	5. $K_2Pt(CN)_4 \cdot xH_2O$	5. 377.36	5. 3.6	5. 6.7	5. 8.7
6. Dichloro(ethylenediamine)platinum(II)	6. n/a	6. $PtCl_2(H_2NCH_2CH_2NH_2)$	6. 326.10	6. 5.0	6. 6.5	6. 8.0
7. Diammino Platinum Dinitrite	7. Dinitritodiamine platinum (II)	7. $Pt(NH_3)_2(NO_2)_2$	7. 321.00	7. 6.5	7. 7.2	7. 7.8
8. Potassium tetrabromoplatinate(II)	8. n/a	8. K_2PtBr_4	8. 592.93	8. 4.2	8. 6.0	8. 8.0
9. Potassium hexabromoplatinate(IV)	9. n/a	9. K_2PtBr_6	9. 752.72	9. 6.5	9. 6.5	9. 6.5
10. Platinum potassium iodide	10. Potassium hexaiodoplatinate(IV)	10. K_2PtI_6	10. 1034.70	10. 5.0	10. 6.9	10. 7.6
11. Platinum potassium thiocyanate	11. Potassium hexathiocyanato platinate (IV)	11. $K_2Pt(CNS)_6$	11. 621.00	11. 7.0	11. 7.4	11. 7.7
12. Di-μ-iodobis(ethylenediamine)diplatinum(II) nitrate	12. PIP	12. $[Pt_2I_2(H_2NCH_2CH_2NH_2)_2](NO_3)_2$	12. 888.20	12. 5.5	12. 5.8	12. 6.0

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Heavy Atom Screen Au - Catalog Number: HR2-444

Name	Synonym	Formula	MW	pH Min	pH Mean	pH Max
1. Gold(I) potassium cyanide	1. Potassium dicyanoaurate (I)	1. $KAu(CN)_2$	1. 288.33	1. 4.2	1. 6.7	1. 8.7
2. Potassium tetrachloroaurate(III) hydrate	2. Gold (III) chloride potassium chloride double salt	2. $KAuCl_4 \cdot xH_2O$	2. 377.88	2. 4.4	2. 6.5	2. 8.0
3. Sodium tetrachloroaurate(III) dihydrate	3. n/a	3. $NaAuCl_4 \cdot 2H_2O$	3. 397.80	3. 6.7	3. 7.5	3. 8.0
4. Gold(III) chloride	4. Auric trichloride	4. $AuCl_3$	4. 303.33	4. n/a	4. n/a	4. n/a
5. Hydrogen tetrachloroaurate(III) trihydrate	5. Hydrogen tetrachloroaurate (III)	5. $HAuCl_4 \cdot 3H_2O$	5. 393.83	5. n/a	5. n/a	5. n/a
6. Potassium tetrabromoaurate(III) dihydrate	6. Potassium gold tetrabromide hydrate	6. $KAuBr_4 \cdot 2H_2O$	6. 591.71	6. 6.3	6. 6.3	6. 6.3

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Heavy Atom Screen Hg - Catalog Number: HR2-446

Name	Synonyms	Formula	MW	pH Min	pH Mean	pH Max
1. Mersalyl acid	1. 2-(3-Hydroxymercurio-2-methoxypropyl carbamoyl)phenoxyacetic acid, 2-[N-(3-Hydroxymercuri-methoxypropyl)-carbamoyl]phenoxyacetic acid, Salyrganic acid	1. $C_{13}H_{17}HgNO_6$	1. 483.87	1. n/a	1. n/a	1. n/a
2. Ethyl Mercuric Phosphate	2. Ethyl mercury phosphate	2. $C_2H_5HgOH_2PO_3$	2. 326.64	2. n/a	2. n/a	2. n/a
3. Mercury(II) chloride	3. n/a	3. $HgCl_2$	3. 271.50	3. 4.2	3. 6.8	3. 9.5
4. Mercury(II) acetate	4. n/a	4. $Hg(OOCCH_3)_2$	4. 318.70	4. 2.8	4. 6.6	4. 8.5
5. Ethylmercurithiosalicylic acid, sodium salt	5. Thimerosal, Merthiolate sodium	5. $C_9H_9HgNaO_2S$	5. 404.80	5. 5.4	5. 6.8	5. 8.4
6. Phenylmercury acetate	6. Mercury phenyl acetate	6. $C_8H_8HgO_2$	6. 336.74	6. n/a	6. n/a	6. n/a
7. Mercury(II) potassium iodide	7. n/a	7. K_2HgI_4	7. 786.48	7. 2.0	7. 6.4	7. 9.3
8. p-Chloromercuribenzoic acid	8. 4-(Chloromercurio)benzoic acid, 4-(Hydroxymercuri)benzoic acid	8. $C_7H_5ClHgO_2$	8. 357.16	8. n/a	8. n/a	8. n/a
9. Ethylmercury chloride	9. Ethylmercuric chloride	9. C_2H_5HgCl	9. 265.13	9. 5.0	9. 6.2	9. 7.0
10. Mercury(II) bromide	10. Mercuric bromide, Mercury dibromide	10. $HgBr_2$	10. 360.44	10. 4.1	10. 6.2	10. 8.0
11. Mercury(II) iodide	11. Mercury diiodide, Mercuric iodide, red mecuric iodide.	11. HgI_2	11. 454.45	11. 2.8	11. 5.7	11. 7.3
12. Mercury(II) nitrate monohydrate	12. Nitric acid, Mercury (+2) salt monohydrate	12. $Hg(NO_3)_2 \cdot H_2O$	12. 324.60	12. n/a	12. n/a	12. n/a
13. Mercury(II) cyanide	13. Dicyanomercury, Mercury dicyanide	13. $Hg(CN)_2$	13. 252.65	13. 6.7	13. 7.3	13. 8.4
14. Mercury(II) oxide, yellow	14. Mercuric oxide, Mercury(2+) oxide	14. HgO	14. 216.59	14. 6.5	14. 6.5	14. 6.5
15. Tetrakis(acetoxymercuri)methane	15. Carbon tetra(acetoxymercuride)	15. $C(HgOOCCH_3)_4$	15. 1050.55	15. 6.0	15. 6.5	15. 8.0

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Heavy Atom Screen M1 - Catalog Number: HR2-448

Name	Synonyms	Formula	MW	pH Min	pH Mean	pH Max
1. Thallium(III) chloride hydrate	1. Thallic chloride, hexahydrate	1. $TlCl_3 \cdot xH_2O$	1. 310.74	1. n/a	1. n/a	1. n/a
2. Thallium(I) chloride	2. Thallium monochloride, Thallous chloride	2. TlCl	2. 239.84	2. n/a	2. n/a	2. n/a
3. Thallium(III) acetate hydrate	3. Thallium triacetate Thallic acetate	3. $Tl(O_2C_2H_3)_3 \cdot xH_2O$	3. 381.52	3. n/a	3. n/a	3. n/a
4. Lead(II) acetate trihydrate	4. Acetic acid, lead(2+)salt trihydrate, Bis(acetato)trihydroxytrilead	4. $Pb(CH_3COO)_2 \cdot 3H_2O$	4. 379.35	4. 4.0	4. 5.6	4. 7.0
5. Lead(II) nitrate	5. Lead dinitrate, Nitric acid, lead(2+) salt, Plumbous nitrate	5. $Pb(NO_3)_2$	5. 331.23	5. 4.5	5. 6.5	5. 7.0
6. Lead(II) chloride	6. Lead(2+) chloride, Lead dichloride, Plumbous chloride	6. $PbCl_2$	6. 278.12	6. 7.5	6. 7.5	6. 7.5
7. Silver nitrate	7. Lunar caustic, Nitric acid, silver(1+)salt	7. $AgNO_3$	7. 169.87	7. 4.5	7. 6.3	7. 8.0
8. Cadmium chloride hydrate	8. Cadmium dichloride hydrate	8. $CdCl_2 \cdot xH_2O$	8. 183.32	8. n/a	8. n/a	8. n/a
9. Cadmium iodide	9. Cadmium Diiodide	9. CdI_2	9. 366.22	9. 6.5	9. 6.5	9. 6.5
10. Potassium hexachloroiridate(IV)	10. Dipotassium iridium hexachloride	10. K_2IrCl_6	10. 483.13	10. 5.7	10. 6.6	10. 7.5
11. Iridium(III) chloride hydrate	11. Iridium trichloride hydrate	11. $IrCl_3 \cdot xH_2O$	11. 298.57	11. 5.8	11. 6.8	11. 8.0
12. Sodium hexachloroiridate(III) hydrate	12. Disodium hexachloroiridate	12. $Na_3IrCl_6 \cdot xH_2O$	12. 473.90	12. 7.0	12. 8.5	12. 9.3
13. Ammonium hexachloroiridate(III) hydrate	13. Triammonium hexachloroiridate (III) hydrate, Triammonium iridium hexachloride hydrate	13. $(NH_4)_3IrCl_6 \cdot xH_2O$	13. 459.05	13. 4.1	13. 5.6	13. 7.0
14. Potassium hexanitroiridium(III)	14. n/a	14. $K_3Ir(NO_2)_6$	14. 585.54	14. 6.9	14. 6.9	14. 6.9
15. Potassium osmate(VI) dihydrate	15. Osmic acid dipotassium salt	15. $K_2OsO_4 \cdot 2H_2O$	15. 368.46	15. 4.3	15. 6.2	15. 7.5
16. Ammonium hexabromoosmate(IV)	16. Diammonium hexabromoosmate (IV)	16. $(NH_4)_2OsBr_6$	16. 705.74	16. n/a	16. n/a	16. n/a
17. Potassium hexachloroosmate(IV)	17. Dipotassium hexachloroosmate	17. K_2OsCl_6	17. 481.15	17. 4.7	17. 5.2	17. 5.8
18. Osmium(III) chloride hydrate	18. Osmium trichloride	18. $OsCl_3 \cdot xH_2O$	18. 296.60	18. 5.0	18. 5.0	18. 5.0
19. Acetoxytrimethyllead(IV)	19. n/a	19. $CH_3CO_2Pb(CH_3)_3$	19. 311.37	19. n/a	19. n/a	19. n/a

Heavy Atom Screens™

HAMPTON RESEARCH
Solutions for Crystal Growth

User Guide (pg 10)

Heavy Atom Screen M2 - Catalog Number: HR2-450

	Name	Synonyms	Formula	MW	pH Min	pH Mean	pH Max
1.	Sodium tungstate dihydrate	1. Tungstic acid disodium salt dihydrate	1. $Na_2WO_4 \cdot 2H_2O$	1. 329.86	1. 4.5	1. 6.2	1. 7.2
2.	Ammonium tetrathiotungstate(VI)	2. Ammonium thiotungstate (VI)	2. $(NH_4)_2WS_4$	2. 348.18	2. n/a	2. n/a	2. n/a
3.	Samarium(III) chloride hexahydrate	3. Samarium trichloride, hexahydrate	3. $SmCl_3 \cdot 6H_2O$	3. 364.80	3. 4.5	3. 6.4	3. 7.0
4.	Samarium(III) acetate hydrate	4. Acetic acid, samarium(+3) salt, hydrate	4. $Sm(O_2C_2H_3)_3 \cdot xH_2O$	4. 327.53	4. 6.2	4. 6.6	4. 7.0
5.	Samarium(III) nitrate hexahydrate	5. Nitric acid, samarium(3+) salt, hexahydrate, Samarium trinitrate hexahydrate	5. $Sm(NO_3)_3 \cdot 6H_2O$	5. 444.47	5. 4.9	5. 6.5	5. 7.5
6.	Lanthanum(III) nitrate hexahydrate	6. Nitric acid, lanthanum(3+) salt, hexahydrate	6. $La(NO_3)_3 \cdot 6H_2O$	6. 433.02	6. n/a	6. n/a	6. n/a
7.	Europium(III) nitrate hexahydrate	7. Nitric acid, europium(3+) salt, hexahydrate	7. $Eu(NO_3)_3 \cdot 6H_2O$	7. 446.07	7. n/a	7. n/a	7. n/a
8.	Europium(III) chloride hexahydrate	8. Europium trichloride, hexahydrate	8. $EuCl_3 \cdot 6H_2O$	8. 366.41	8. 5.0	8. 5.2	8. 5.5
9.	Gadolinium(III) chloride hydrate	9. Gadolinium trichloride	9. $GdCl_3 \cdot xH_2O$	9. 263.61	9. n/a	9. n/a	9. n/a
10.	Lutetium(III) chloride hexahydrate	10. Lutetium trichloride, hexahydrate	10. $LuCl_3 \cdot 6H_2O$	10. 389.42	10. 5.0	10. 5.2	10. 5.5
11.	Lutetium(III) acetate hydrate	11. Acetic acid, lutetium(+3) salt, hydrate	11. $Lu(O_2C_2H_3)_3 \cdot xH_2O$	11. 352.11	11. n/a	11. n/a	11. n/a
12.	Ytterbium(III) chloride hydrate	12. Ytterbium trichloride	12. $YbCl_3 \cdot xH_2O$	12. 279.40	12. n/a	12. n/a	12. n/a
13.	Dysprosium(III) chloride hexahydrate	13. Dysprosium trichloride, hexahydrate	13. $DyCl_3 \cdot 6H_2O$	13. 376.95	13. 5.5	13. 5.8	13. 6.2
14.	Praseodymium(III) chloride heptahydrate	14. Praseodymium trichloride, heptahydrate	14. $PrCl_3 \cdot 7H_2O$	14. 373.37	14. 7.5	14. 7.5	14. 7.5
15.	Neodymium(III) chloride hydrate	15. Neodymium trichloride, hexahydrate	15. $NdCl_3 \cdot xH_2O$	15. 250.60	15. 4.9	15. 6.1	15. 8.7
16.	Holmium(III) chloride hexahydrate	16. Holmium trichloride	16. $HoCl_3 \cdot 6H_2O$	16. 379.38	16. 5.5	16. 5.5	16. 5.5
17.	Potassium hexachlororhenate(IV)	17. Dipotassium hexachlororhenate	17. K_2ReCl_6	17. 477.12	17. 4.3	17. 5.8	17. 8.0
18.	Potassium perrhenate	18. Potassium rhenate ($KReO_4$), Potassium rhenium oxide	18. $KReO_4$	18. 289.30	18. 7.5	18. 7.5	18. 7.5
19.	Sodium phosphotungstate tribasic hydrate	19. Tri-Sodium phosphotungstate, Phosphotungstic acid trisodium salt hydrate, Tungstophosphoric acid trisodium salt	19. $Na_3[P(W_3O_{10})_4] \cdot aq$	19. 2946.00	19. n/a	19. n/a	19. n/a

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