

Isolation/Modification/Labeling

Chelate & Metal chemistry

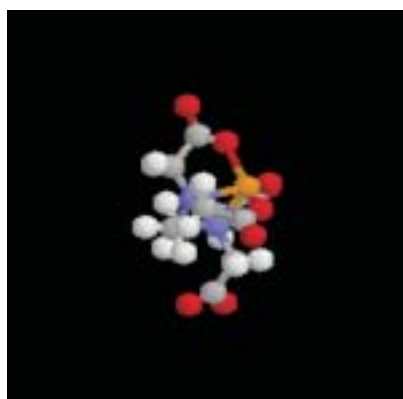
EDTA & analogs chelating agents

Chelating agents are organic compounds that are used to trap metal ion in circular structures (chelate circles) by several coordination bounds. Most include oxygen, nitrogen and (or) sulfur, and are bases on ethylenediamine, acetyl acetone, or oxine. EDTA is popular because it is very stable. These chelating agents are used for titration (colorimetry, fluorimetry), isolation and separation of metal ions. They are also used in masking of certain ions, solubilization of metals in organic solvents, gas chromatography, of metal ions.

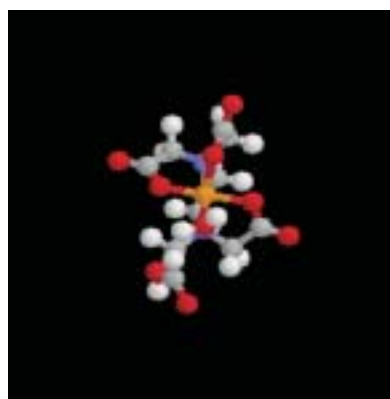
Metal indicators are chelating reagents that can be used to colorimetrically or fluorometrically determine metal ion concentration in solutions. Acetyl acetone (AA) and its analogs are utilized for solvent extractions of metal ions from aqueous solutions. These metal complexes are used as catalysts of polymerization, dryness and combustion.

Chelating reagents, including EDTA, EDTA analogs, metal salts and others, are available in bulk quantities. Please inquire for specifications, technical information (stability constants).

Chelate structures with five or six member rings form the most stable chelate circle. In chelating reactions of typical chelating agents, such as ethylenediamine, acetyl acetone and oxine, several molecules are coordinated with one metal ion. Ethylenediamine tetraacetic acid (EDTA), which has many coordinated atoms, forms a very stable chelate between one molecule of EDTA and metal ion.



Complex with EDTA as a pentadentate ligand



Octahedral complex with EDTA and water

Chelating Agents / EDTA

Name	Cat.#	Qty	MW	Application	Solubility
4H(EDTA.free acid)	T31710	500 g	292.24	Chelate titration, metal masking, metal isolation	34 mg/100ml water
2Na(EDTA.2Na)	T32140	500 g	372.24	Chelate titration, metal masking, metal isolation	11.1 g/100ml water
3Na(EDTA.3Na)	R49090	500 g	472.23	Chelate titration, metal masking, metal isolation	46.5 g/100 ml water
4Na(EDTA.4Na)	T32160	500 g	452.23	Chelate titration, metal masking, metal isolation	60 g/100 ml water
2K(EDTA.2K)	T31910	50 g	404.45	Chelate titration, metal masking, metal isolation	100 g/100 ml water
3K(EDTA.3K)	T31920	50 g	442.54	Chelate titration, metal masking, metal isolation	100 g/100 ml water
2NH4(EDTA.2NH4)	T32180	500 g	326.3	Chelate titration, metal masking, metal isolation	5 g/100ml water
Ca(II)-EDTA	T31340	50 g	410.3		
Cu(II)-EDTA	T31360	25 g	469.8		
Fe(III)-EDTA	T31370	50 g	421.09		
Mg(II)-EDTA	T31380	25 g	430.56		
Zn(II)-EDTA	T31400	25 g	471.64		

Chelating Agents/ EDTA Analogs

Name	Cat.#	Qty	MW	Application	Solubility
CyDTA	T30610	25 g	364.35	Metal masking	
DTPA	T31040	5 g	393.35	Chelating agent	
EDDP	T31320	5 g	277.15	Chelate titration, metal masking, metal isolation	1 g/100ml water
EDTA-OH	T31330	5 g	278.26	Chelate titration, metal masking, metal isolation	
GEDTA (EGTA)	T31560			Chelating agent	
HIDA	T31730	5 g	177.16	Chelating agent	1 g/100ml water
IDA	T31860	25 g	133.1	Intermediate of chelating agent synthesis	1 g/100ml water
NTA	T32240	500 g	191.14	Metal masking, metal isolation	
NTPO	T32290	5 g	365	Chelate titration, metal masking, metal isolation	2 g/100 ml water
TTHA	T33110	5 g	494.45	Chelate titration, metal masking, metal isolation	

Metals indicators

There are several methods for measuring a particular metal ion in solution, including :

- ◆ Chelate titration
- ◆ Colorimetric detection
- ◆ Fluorometric detection
- ◆ Colorimetric detection coupled with solvent extraction
- ◆ Precipitation titration.

Chelate Titration

Metal indicators and chelating agents are used to determine the concentration of specific metal ions in solution by chelate titration because the colour of the metal indicator varies sharply with the association and dissociation of metal ions. EDTA forms a 1:1 complex with most metal ions that are divalent or more. EDTA-metal complexes are very stable and have high dissociation constants. For these reasons, EDTA is a widely used titration reagent.

Fluorescent metal indicators are useful for determining the titration endpoint of metal ions in stained samples.

Spectrophotometry

Colorimetric chelating reagents form coloured complexes with metal ions in pH-controlled solutions. Their selectivity depends on the dissociation constants of metal ions and their sensitivity depends on the molar absorptivity of the complex. However, few colorimetric chelating reagents are highly selective. To increase selectivity, the choice of masking reagents or solvents for the extraction procedures is important. The maximum wavelength of the complex is also an important factor for selectivity and sensitivity. For example, Nitroso-PSAP forms complexes with several heavy metal ions, but the maximum wavelength of the Nitroso-PSAP-Fe complex is considerably longer than that of the other metal complexes. Thus, iron can be determined without interference from other metal ions. Water-soluble colorimetric chelating agents enable the determination of metal ions in aqueous solution without solvent extraction. Therefore, these reagents are useful for automatic detection systems.

Masking Reagent

EDTA forms stable complexes with various metal ions in chelate titration. The total consumption of EDTA solution indicates the total amount of mixed metal ions contained in the sample solution. To determine the amount of one specific metal ion in the sample solution, masking reagents should be added to remove other metal ions.

Reagents for Ion Selective Electrodes

Real-time monitoring of electrolytes is increasingly important for clinical use. For example, monitoring sodium and potassium ion concentrations in the blood flow is essential during cardiac surgery. Although lithium ion is used in the treatment of manic symptoms, its serum level must be strictly monitored due to its toxicity. For the simple and quick determination of these alkaline and alkaline earth metal ions, polyvinyl chloride (PVC) membrane electrodes have been widely used. The concentration of neutral carriers, plasticizers, and counter-anions used to prepare the PVC electrode determines its ion selectivity. A large number of crown ether compounds have been developed. Some of them are superior to naturally existing neutral carriers such as valinomycin, which is highly selective for potassium ions.

These methods use several metal reagents to chelate metal ions, mask, or detect by a colour modification or fluorescence upon binding with metals. In general, metal indicators are utilized for chelating titration and colorimetry, while fluorometric chelating agents are utilized for the determination of the metal concentration by spectrophotometry.

The following table displays metal indicators for these applications, including fluorimetry, chelatometry and colorimetry. Chemical product names and CAS number can be found in alphabetic index and CAS index, or at <http://www.interchim.com/interchim/customers/default.cfm>

Example of product description : 5-Br-PSAA #T30290

2-(5-Bromo-2-pyridylazo)-5-[N-propyl-N-(3-sulfopropyl)amino]aniline, sodium salt

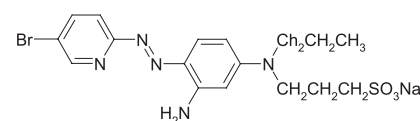
CAS Number: 86035-60-7

Absorbance (1.03×10^{-5} M in buffer soln.): >0.40 (458 nm)

Molar absorptivity (Fe complex): >86 000 (558 nm)

Solubility: 5 mg/10 ml water

5-Br-PSAA is a water-soluble colorimetric reagent for Fe(II) and Co(III) detection. This reagent forms colored complexes with Fe, Ni, Cu and Co, but not with Zn. The Fe(II) and Co(III) complexes are very stable, and even EDTA cannot remove metals from these complexes. However, Cu(II) and Ni(II) complexes are decomposed by EDTA, so 5-Br-PSAA can be used to determine Fe(II) in the presence of Cu(II) or Ni(II). The 5-Br-PSAA assay is 4 times as sensitive as Bathophenanthroline assay. Dr. Sakai and others determined ppb levels of Pb (EC=98,400) using 5-Br-PSAA by flow injection analysis. Dr. Makino and others determined Cu(II) in 0.2 ml of serum and urine by direct colorimetric detection (max=580 nm, EC=64,000).



S-Br-PSAA literature

Clin Chim Acta. 1989 Oct 31;185(1):7-16; Makino T.; A sensitive, direct colorimetric assay of serum copper using 5-Br-PSAA.

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Name	MW	Application	Ca	Co	Cu	Fe	Mg	Ni	Zn	Others	Cat.#	Qty
ALC	385.32	colorimetric det.								F ⁻	S29830	1 g
3,5-DiBr-PAESA	546.21	colorimetric det.			Cu					Ag	47466	100 mg
5-Br-PAPS	537.34	colorimetric det.		Co	Cu			Ni	Zn	Pd, Pt, Rh, Ru, Zn, Pb	204970	100 mg
5-Br-PSAA	478.34	colorimetric det.		Co		Fe					T30290	100 mg
Alfusone		colorimetric det.								F ⁻	S59460	25 g
Arsemate	256.14	colorimetric det.								Sb, As	559620	5 g
Azomethine H	467.38	colorimetric det.									560760	5 g
Bathocuproindisulfonic acid	564.54	colorimetric det.			Cu						T28650	1 g
Bathocuproine	360.45	colorimetric det. by solvent extraction			Cu						BM1600	100 mg
Bathophenanthroline	322.40	colorimetric det. by solvent extraction			Cu	Fe				Ru	T28820	1 g
Bathophenanthrolinedisulfonic acid	536.49	colorimetric det.			Cu	Fe					T29190	1 g
Bis(12-crown-4)		ionophore								Na	BM1620	100 mg
Bis(benzo-15-crown-5)	720.80	ionophore								K	714515	100 mg
Bismuthiol-II	264.44	colorimetric det. by solvent extraction								As, Bi, Os, Re, Te	T29960	1 g
Bisthiourea-1	582.91	colorimetric det. by solvent extraction								Cl ⁻	T30550	25 mg
BT	461.38	colorimetric det.	Ca	Co			Mg		Zn	Cd, Hg, Pb	T30230	25 g
C14-K22B5	897.28	ionophore					Mg				T30780	10 mg
Calcein	622.53	fluorometric det.	Ca		Cu		Mg		Zn	Al, Ba	FP-466251	100 mg
Calcein Blue	321.28	fluorometric det.	Ca	Co	Cu	Fe		Ni		Ba, Cr, F, Sr, Zr	111416	1 g
Cesibor	450.21	Precipitation reagent								Cs	T30580	1 g
Chlorophosphonazo-III	801.33	colorimetric det.	Ca				Mg			Ac, Ba, Gd, La, Nd, Np, Pa, Pu, Rare earth metals, Sc, Sr, Th, Ti, U, Zr	114238	100 mg
Chromotropic acid	400.29	colorimetric det.				Fe				B, NH ⁴⁺ , Th, Ti, U, Zr	114801	5 g
Co(III)-5-Cl-PADAP	701.92	colorimetric det. by solvent extraction									BE8200	100 mg
Cu-PAN		Metal indicator	Ca	Co	Cu	Fe	Mg	Ni	Zn	Al, Ga, Hg, In, V	T30590	10 g
Cyanoline Blue		colorimetric det.								CN ⁻ , NH ⁴⁺ , OCN ⁻ , SCN ⁻	T30600	25 g
DAB	360.11	colorimetric, peroxidase fluorimetric det.								Se, V	01012D	1 g
DAN	158.20	Colorimetric and fluorometric det.								NO ₂ ⁻ , SE	T31060	1 g
Diantipyrylmethane	406.48	colorimetric det.				Fe				Mo, Ti, U	T30980	25 g
Dibenzyl-14-crown-4	384.51	ionophore								Li	310900	50 mg
HDOPP-Ca	987.29	ionophore	Ca								T31726	1 g
HNB	620.48	colorimetric det.	Ca							Ba, Rare earth metals, UO ₂	T31740	1 g
HFPB	1836.65	lipophilic anion									T31800	100 mg
Ionophore-K23E1	1041.53	ionophore									T30470	25 mg
Kalibor	342.22	Precipitation reagent								K	T31930	25 g
K-TCPB	496.10	Lipophilic anion, counter anion for ion selective electrode									T31941	1 g
Murexide	284.19	colorimetric det.	Ca							Rare earth metals	14039C	5 g
MX		colorimetric det.	Ca							Rare earth metals	T32020	500 g
Nitro-PAPS	503.45	colorimetric det.		Co	Cu			Ni	Zn		281000	100 mg
Nitroso-PSAP	302.35	colorimetric det.									T32200	100 mg
NN	438.41	colorimetric det.	Ca							UO ₂	T32230	5 g
NN diluted with potassium sulfate		colorimetric det.									T32220	25 g
o-Phenanthroline	198.22	colorimetric det.								Ag	T32630	5 g
PAN	249.27	colorimetric det.		Co	Cu	Fe		Ni	Zn	Os, Rare earth metals	F23963	1 g
PAR	215.21	colorimetric det. by solvent extraction		Co				Ni	Zn	Bi, Ga, V	T32590	1 g
PC (Phthalein Complexone)	636.60	colorimetric det.	Ca				Mg			Ba, Hg, La, Sr	T32600	1 g
PR (Pyrogallol Red)	400.36	colorimetric det.		Co	Cu					Al, Ga, Ge, Ti	T32660	1 g
SATP	229.30	colorimetric det. by solvent extraction			Cu			Ni		Sn	T32850	1 g
Sodium Bicinchoninate	388.28	colorimetric det.			Cu						T30320	5 g
TD19C6	602.88	ammonium selective electrode								NH ₄ ⁺	T33210	10 mg
tert-HDOPP-Ca	987.29	ionophore	Ca								T31770	1 g
TFPB		lipophilic anion									736933	100 mg
Tiron		colorimetric det.									06339D	5 g
TMPyP	1363.61	colorimetric det.			Cu						T32990	100 mg
Topo	386.63	solvent extraction									704734	25 g
TPPS		colorimetric det.		Co	Cu					Pb	T3300	100 mg
XB-I	513.50	colorimetric det.									T33260	1 g
XO (Xylenol Orange)	716.62	colorimetric det., metal indicator							Zn	Al, Bi, Nb, OU,	T33270	1g
Zephiramine	404.07	detection									T33280	5 g
Zincon	462.41	colorimetric det.	Ca		Cu				Zn	Cd, Hg, Pb	E44556	1 g

For more information about these ion detectors, please contact us.