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Volatile Precursors for NanoFabrication

Vol. 4 No. 3

ALD Precursors for High κ and Barrier Materials

Precursors for Low κ Materials

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Precursors for Nanofabrication: For Your Lab or for Your Fab

Sigma-Aldrich is pleased to present our complete line of high-purity organometallics and inorganics for micro and nanoelectronic applications. In this brochure you will find products for all aspects of atomic layer (ALD) and chemical vapor deposition (CVD). We feature precursors for high and low (κ) dielectric materials, transition metals for barrier and metallization applications, III-V materials, and epitaxy gases. This brochure features a discussion of the ALD process and technical synopses on key application areas, equipment, books and software of interest to researchers and engineers.

Ready to begin? Look through our product index below by end material type and then go to the page to find the products you need. Do you have a precursor in mind but can't find it in this brochure? Need a precursor for a rare-earth oxide or a single source nitride precursor? Contact our Organometallics Product Manager at **matsci@sial.com**.

Material Deposited	Product Name	Page
Al_2O_3, Al, AlN, AlP AlAs, $LaAlO_3$, Aluminates	Aluminum *sec*-butoxide	2
	Aluminum tribromide	6
	Aluminum trichloride	6
	Diethylaluminum ethoxide	2
	Tris(ethylmethylamido)aluminum	2
	Triethylaluminum	2
	Triisobutylaluminum	2
	Trimethylaluminum	2
	Tris(diethylamido)aluminum	2
	Tris(ethylmethylamido)aluminum	2
AlAs, GaAs, InAs	Trimethylarsine	8
MgB_2, BN, B, B_4C, B_2O_3 B doping	Diborane (10% in Hydrogen)	10
	Diborane-d_6 (10% in D_2 or He)	10
	Trimethylboron	10
	Trimethylboron-d_9	10
Co, CoO, $CoSi_2$	Bis(N,N'-Diisopropylacetamidinato)cobalt(II)	4
	Dicarbonyl(cyclopentadienyl)cobalt(I)	9
Cu, $YBaCuO_x$, CuO	(N,N'-Diisopropylacetamidinato)copper(I)	4
Fe, FeO	Bis(N,N'-di-tert-butylacetamidinato)iron(II)	4
Ga_2O_3, Ga, GaN, GaP, GaAs	Gallium tribromide	6
	Gallium trichloride (bead or slug)	6
	Triethylgallium	7
	Triisopropylgallium	7
	Trimethylgallium	7
	Tris(dimethylamido)gallium	7
	Tri-*tert*-butylgallium	7
Ge, GeO_2, GeSi	Digermane (10% in H_2)	10
	Germane	10
	Tetramethylgermanium	10
HfO_2, Hf_3N_4	Hafnium(IV) chloride	6
	Hafnium(IV) *tert*-butoxide	2
	Tetrakis(diethylamido)hafnium(IV)	2
	Tetrakis(dimethylamido)hafnium(IV)	2
	Tetrakis(ethylmethylamido)hafnium(IV)	2
In_2O_3, InN, InP, InAs In containing Solar Cells Indium Tin Oxide	Indium trichloride	6
	Indium(I) iodide (Anhydrous beads)	6
	Indium acetylacetonate	7
	Triethylindium	7
La_2O_3, $LaAlO_3$	Tris(N,N'-Di-tert-butylacetamidinato)lanthanum(III)	4
Mg dopant in III-V	Bis(pentanethylcyclopentadienyl)magnesium	9
MoS_2, MoO_2, Mo	Molybdenum hexacarbonyl	6
	Molybdemum(V) chloride	6
	Molybdenum(VI) fluoride	6
GaN, InGaN, AlGaN, Si_3N_4	N,N-dimethylhydrazine	8
	Ammonia	8
	Azidotrimethylsilane	8
Nb_2O_5	Niobium(V) chloride	6
	Niobium(V) ethoxide	9
Ni, NiO	Bis(methylcyclopentadienyl)nickel(II)	9
P doping, InP, GaP	Phosphine	10
	Phosphine-d_3	10
	tert-Butylphosphine	8
	Tris(trimethylsilyl)phosphine	8
Pt, PtO_2	Cyclopentadienyl(trimethyl)platnium(IV)	9
Ru, RuO_2	Bis(ethylcyclopentadienyl)ruthenium(II)	9
Sb Source	Trimethylantimony	8
	Tris(dimethylamido)antimony	8
$SiO_2/Si_3N_4/SiC$	2,4,6,8-Tetramethylcyclotetrasiloxane	4
	Dimethoxydimethylsilane	4
	Disilane	10
	Methylsilane	10
	Octamethylcyclotetrasiloxane	4
	Silane	10
	Silane-d_4	10
	Tris(isopropoxy)silanol	4
	Tris(*tert*-butoxy)silanol	4
	Tris(*tert*-pentoxy)silanol	4
Ta_2O_5/TaN	Pentakis(dimethylamido)tantalum(V)	9
	Tantalum(V) chloride	6
	Tantalum(V) ethoxide	9
	Tris(diethylamino)(*tert*-butylimido)-tantalum(V)	9
TiN/TiO_2	Bis(diethylamido)bis(dimethylamido)-titanium(IV)	3
	Tetrakis(diethylamido)titanium(IV)	3
	Tetrakis(dimethylamido)titanium(IV)	3
	Tetrakis(ethylmethylamido)titanium(IV)	3
	Titanium(IV) bromide	6
	Titanium(IV) chloride	6
	Titanium(IV) *tert*-butoxide	3
V_2O_5	Vanadium(V) oxytriisopropoxide	9
W, WO_2, WO_3, WC	Bis(*tert*-butylimido)bis(dimethylamido)-tungsten(VI)	9
	Tungsten hexacarbonyl	6
	Tungsten(VI) chloride	6
	Tungsten(VI) fluoride	6
Y_2O_3, YBaCuOx	Tris(N,N-bis(trimethylsilyl)amide)yttrium(III)	9
	Yttrium(III) butoxide solution 0.5M in toluene	9
ZnO	Diethylzinc	9
Zr_3N_4, ZrO_2	Tetrakis(diethylamido)zirconium(IV)	3
	Tetrakis(dimethylamido)zirconium(IV)	3
	Tetrakis(ethylmethylamido)zirconium(IV)	3
	Zirconium(IV) bromide	6
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	Zirconium(IV) *tert*-butoxide	3

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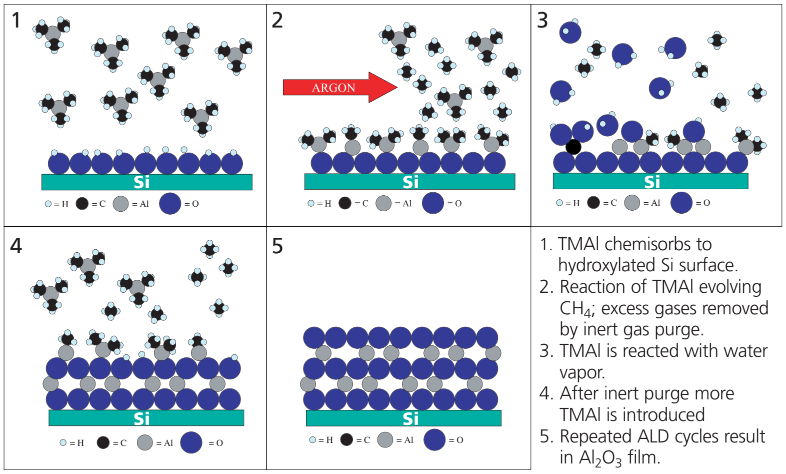
Atomic Layer Deposition

Atomic Layer Deposition (ALD) is recognized as the key technology for the semiconductor industry to break below the 90 nm device node barrier, keeping device miniaturization on track with Moore's Law.[1] ALD processes can be used for the deposition of barrier materials,[2] nucleation layers, metallization,[3] and high κ dielectrics.[4] The ALD process is able to meet the demands of microelectronics miniaturization because it is a layer-by-layer build up of materials starting with the chemisorption of molecular precursors (Figure). These precursors are reacted at the substrate surface and the resulting layer is purged of by-products with inert gas.[5] The process is repeated as needed to attain desired film characteristics. Because ALD is a self-limiting deposition process, it offers a high degree of control over film composition, thickness and 100% step-coverage, even over high aspect ratio steps.[6] Contrast this with traditional CVD processes where gas-phase chemical reactions produce the final material to be deposited on the surface. While effective for traditional thick and thin-film applications, CVD does not offer the layer-by-layer control and step coverage of ALD. Furthermore, recent advances in processing technology are allowing for ALD processes to be used in high throughput.



1. TMAl chemisorbs to hydroxylated Si surface.
2. Reaction of TMAl evolving CH_4; excess gases removed by inert gas purge.
3. TMAl is reacted with water vapor.
4. After inert purge more TMAl is introduced
5. Repeated ALD cycles result in Al_2O_3 film.

The ALD mechanism is composed of two separate self-limiting steps: the substrate saturation process and the reactivity between the surface groups and precursor molecules. These requirements place several demands on the ALD precursor molecule. Not every molecule is ideal but we can help you find the material ideal for your application.

Sigma-Aldrich, a leader in *High Technology* products is proud to present our line of Volatile Precursors for Nanofabrication. These products encompass a wide variety of products to get you the final material phases you need.

Ideal ALD Precursor Characteristics

- High vapor pressure
- Thermal stability prior to deposition
- Ease of handling and transfer
- Chemisorbs to substrate
- Aggressive reaction with complementary precursors
- Noncorrosive to substrate
- High purity
- Low hazard by-products

High κ Materials

The miniaturization of integrated devices brings serious challenges to the continued use of current materials. The capacitors used in traditional microelectronic circuits, composed of Si/SiO_2/ metal, will not be able to function due to the physical limits of the SiO_2 dielectric. At the nanometer dimension, the SiO_2 dielectric constant (κ) is not large enough to prevent leakage currents, leading to the unwanted discharge of the capacitor. New higher κ materials are under consideration and are listed in the table. 1.5-10 nm thick layers of Zr, Hf and Al oxides on silicon, grown by ALD processes exhibit much lower gate leakage than SiO_2 of equivalent thickness. Sigma-Aldrich offers a wide array of volatile Al, Hf and Zr precursors for your high κ deposition processes. We can tailor ligand designed to give you the physical properties and purity you demand for your systems.

Candidate High κ Materials

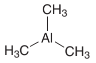
Material	Dielectric constant (κ)
Si_3N_4/SiO_2	5-6
Sc_2O_3	>10
Al_2O_3	8-9
Y_2O_3	15
HfO_2	21
ZrO_2	22
$LaAlO_3$	25
Ta_2O_5	25
La_2O_3	25-30
$SrTiO_3$	200
$Ba_xSr_{1-x}O_3$	300

Precursors for High κ Materials

Aluminum

Trimethylaluminum

J1,0001-3
Purity: 99.99999%
CAS No. 75-24-1
MF: $(C_3H_9)Al$
FW: 72.09
mp: 15 °C
bp: 125–126 °C
Density: 0.752 g/mL

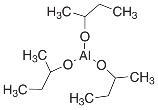


Typical ICP-MS results for J1,0001-3 in ppb

Ag	<1	Ge	3	Pt	<1
As	<1	Hf	8	Sb	<1
Au	<1	Hg	<1	Sn	<1
B	<1	In	<1	Sr	<1
Ba	4	K	<1	Ta	<1
Be	<1	La	<1	Th	<1
Bi	<1	Li	<1	Ti	4
Ca	6	Mg	1	Tl	<1
Cd	<1	Mn	<1	U	<1
Co	<1	Mo	1	V	<1
Cr	3	Na	44	W	<1
Cu	1	Nb	<1	Zn	2
Fe	4	Ni	2	Zr	<1
Ga	<1	Pb	<1		

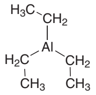
Aluminum *sec*-butoxide

51,160-9
Purity: 99.99%
CAS No. 2269-22-9
FW: 246.33
bp: 200-206 °C @ 30 mmHg
Density: 0.967 g/mL



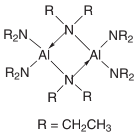
Triethylaluminum

J1,0001-8
Purity: 99.999%
CAS No. 97-93-8
MF: $(C_2H_5)_3Al$
FW: 114.17
mp: -50 °C
bp: 128–130 °C @ 50 mmHg
Density: 0.835 g/mL



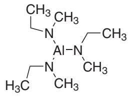
Tris(diethylamido)aluminum

J1,0003-0
CAS No. 352546-72-6
FW: 486.74
mp: 28–31 °C
bp: 50 °C @ 20 mmHg
Density: 0.915 g/mL

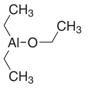


Also Available

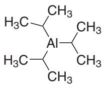
J1,0002-9	**Tris(ethylmethylamido)aluminum**
25,674-9	**Diethylaluminum ethoxide 97%**
25,720-6	**Triisobutylaluminum**



J1,0002-9



25,674-9

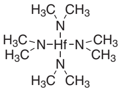


25,720-6

Hafnium

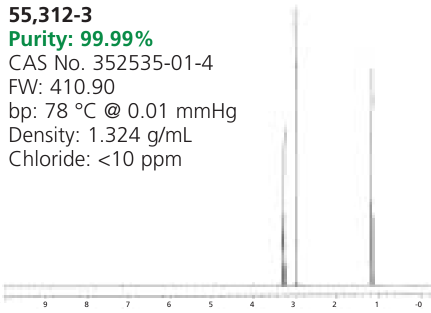
Tetrakis(dimethylamido)hafnium(IV)

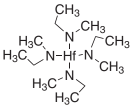
45,519-9
Purity: 99.99%
CAS No. 19962-11-9
FW: 354.80
mp: 26–29 °C



Tetrakis(ethylmethylamido)hafnium(IV)

55,312-3
Purity: 99.99%
CAS No. 352535-01-4
FW: 410.90
bp: 78 °C @ 0.01 mmHg
Density: 1.324 g/mL
Chloride: <10 ppm

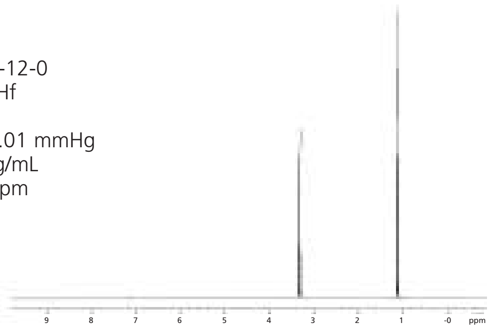




Typical ^1H NMR

Tetrakis(diethylamido)hafnium(IV)

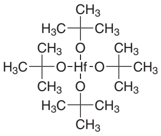
45,520-2
Purity: 99.99%
CAS No. 19962-12-0
MF: $[(C_2H_5)_2N]_4Hf$
FW: 467.01
bp: 130 °C @ 0.01 mmHg
Density: 1.249 g/mL
Chloride: <10 ppm



Typical ^1H NMR

Hafnium(IV) *tert*-butoxide

44,554-1
Purity: 99.99%
CAS No. 2172-02-03
FW: 473.95
bp: 90 °C @ 5 mmHg
Density: 1.166 g/mL

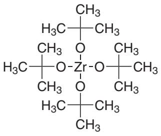


Precursors for High κ Materials—*cont'd*

Zirconium

Zirconium(IV) *tert*-butoxide

56,003-0
Purity: 99.999%
CAS No. 2081-12-1
FW: 383.68
bp: 81 °C @ 3 mmHg
Density: 0.985 g/mL

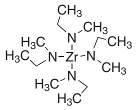


Tetrakis(dimethylamido)zirconium(IV)

57,921-1
Purity: 99.99%
CAS No. 19756-04-8
MF: $[(CH_3)_2N]_4Zr$
FW: 267.53
mp: 57–60 °C

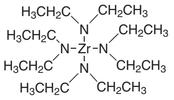
Tetrakis(ethylmethylamido)zirconium(IV)

55,313-1
Purity: 99.99%
CAS No. 175923-04-3
FW: 323.63
bp: 81 °C @ 0.1 mmHg
Density: 1.049 g/mL



Tetrakis(diethylamido)zirconium(IV)

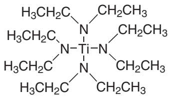
J1,0002-3
Purity: 99.99%
CAS No. 13801-49-5
FW: 379.74
bp: 128 °C @ 0.05 mmHg



Titanium Precursors for Barrier Materials

Tetrakis(diethylamido)titanium(IV)

46,986-6
Purity: 99.99%
CAS No. 4419-47-0
FW: 336.42
bp: 112 °C @ 0.1 mmHg
Density: 0.931 g/mL

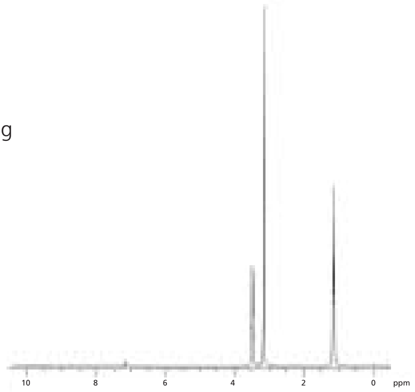


Tetrakis(dimethylamido)titanium(IV)

46,985-8
Purity: 99.999%
CAS No. 3275-24-9
MF: $[(CH_3)_2N]_4Ti$
FW: 224.21
bp: 50 °C @ 05 mmHg
Density: 0.947 g/mL

Tetrakis(ethylmethylamido)titanium(IV)

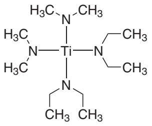
47,353-7
Purity: 99.99%
CAS No. 308103-54-0
MF: $[(CH_3)(C_2H_5)N]_4Ti$
FW: 280.32
bp: 80 °C @ 0.1 mmHg
Density: 0.923 g/mL



Typical ^1H NMR

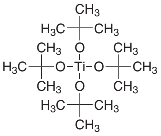
Bis(diethylamido)bis(dimethylamino)titanium(IV)

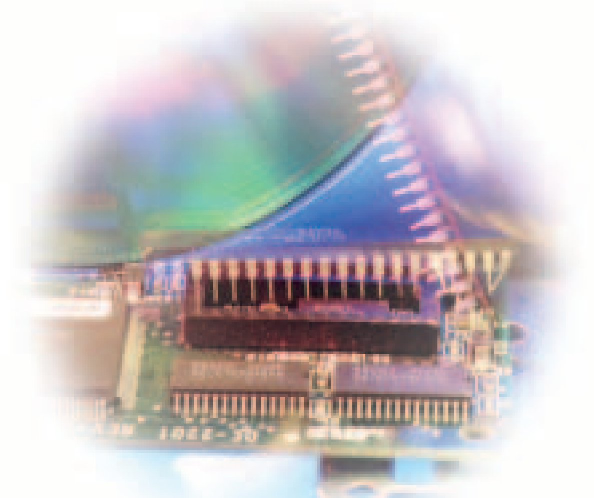
J1,0002-6
Purity: 99.99%
CAS No. 123798-13-0
FW: 280.31
bp: 80 °C @ 0.1 mmHg
Density: 0.931 g/mL



Titanium(IV) *tert*-butoxide

46,255-1
CAS No. 3087-39-6
MF: $[(CH_3)_3CO]_4Ti$
FW: 340.36
bp: 70 °C @ 0.2 mmHg
Density: 0.881 g/mL





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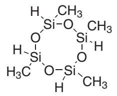
Low κ Precursors

Low κ materials address technical challenges of increased chip performance by allowing for the reduction of spacing between metals in multi-level interconnects, interlayer dielectrics and passivation layers.[8] Shrinking of device sizes leads to issues with resistance capacitance (RC) coupling, resulting in power dissipation, propagation delay and noise between circuits called crosstalk. Current low κ strategies include orgaonsilicate glass (OSG) films for the 90-100 nm node (κ <3), carbon doped silicon oxide films (κ <3), and porous silicate films for the 65 nm node (κ <2.6). Porous films have some copper compatibility issues and reducing the κ of such films is accompanied by a loss of mechanical properties. Future low κ materials will be an extension of current CVD/ALD deposited non-porous films. Sigma-Aldrich has a variety of high quality low κ precursors. If you can't find what you want check the website or send a question to **matsci@sial.com**.

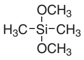
2,4,6,8-Tetramethylcyclotetrasiloxane

51,299-0
Purity: 99.999%
CAS No. 2370-88-9
FW: 240.51
mp: -69 °C
bp: 134 mmHg
Density: 0.986 g/mL
Chloride: <10 ppm



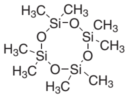
Dimethoxydimethylsilane

55,668-8
Purity: 99.999%
CAS No. 1112-39-6
FW: 120.23
bp: 81.4 °C
Density: 0.880 g/mL



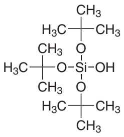
Octamethylcyclotetrasiloxane

23,569-5
Purity: 98+%
CAS No. 556-67-2
FW: 296.62
mp: 17-18 °C
bp: 175-175 °C
Density: 0.956 g/mL



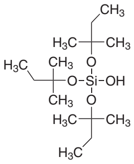
Tris(*tert*-butyoxy)silanol

55,346-8
Purity: 99.999%
CAS No. 18166-43-3
FW: 264.43
mp: 63–65 °C
bp: 205–210 mmHg
Chloride: <50 ppm



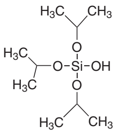
Tris(*tert*-pentoxy)silanol

55,344-1
Purity: 99.99%
CAS No. 17906-35-3
MF: $[(C_2H_5)(CH_3)_2CO]_3SiOH$
FW: 306.51
bp: 96–99 °C @ 2.5 mmHg
Density: 0.944 g/mL
Chloride: <100 ppm



Tris(isopropoxy)silanol

J1,0002-8
Purity: 99%
CAS No. 27491-86-7
MF: $[(CH_3)_2HCO]_3SiOH$
FW: 222.36

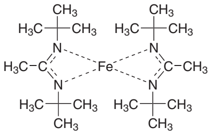


Amidinate Precursors

Developed with Professor Roy Gordon at Harvard, Sigma-Aldrich presents these exciting new precursors for Atomic Layer Deposition. The amidinates are volatile, homoleptic transition metal precursors, which meet the rigorous standards for ALD applications. When employed in ALD processes, these precursors allow for the deposition of pure metals when reacted with H_2 gas or oxides when co-reacted with water vapor.[9] The precursors can be vaporized appreciably at temperatures between 50-100 °C for the transition metal compounds and at 130 °C for the lanthanum compound. Deposition temperatures range between 150-350 °C.

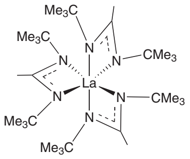
Bis(*N,N'*-di-tert-butylacetamidinato)iron(II)

J1,0000-6
Purity: 99%
CAS No. 635680-56-7
FW: 394.42



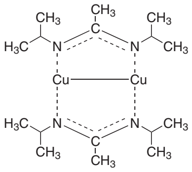
Tris(*N,N'*-Di-tert-butylacetamidinato)lanthanum(III)

J1,0000-8
Purity: 99.999%
FW: 646.77
mp: 165 °C



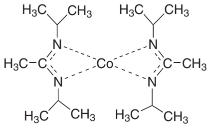
(*N,N'*-Diisopropylacetamidinato)copper(I)

J1,0000-9
Purity: 99%
CAS No. 635680-64-7
FW: 409.56
mp: 152–154 °C



Bis(*N,N'*-Diisopropylacetamidinato)cobolt(II)

J1,0001-0
Purity: 99.98%
CAS No. 635680-58-9
FW: 341.40
mp: 80–83 °C



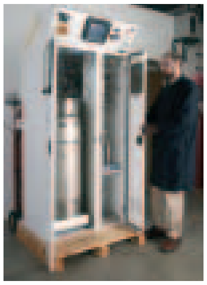
Sigma-Aldrich Fine Chemicals Capabilities:

Manufacturing Capabilities for Volatile Precursors

Sigma Aldrich Fine Chemicals (SAFC) is known as a worldwide leader in the manufacture of high purity chemicals and biotechnology products. We have decades of experience in the production, purification and handling of air-sensitive organometallics at our ISO9001 certified Sheboygan, Wisconsin facility, manufacturing high-purity inorganics through our Aldrich-APL facility in Urbana, Illinois and stable isotope materials at our ISOTEC™ plant in Miamisburg, Ohio. We have translated this expertise into a world-class capability to manufacture a broad range of high technology products. No molecule is beyond our grasp, whether you need a few grams for proof-of-concept or you are ready to go to production, SAFC can provide you with the quality materials you need to get the job done.

SAFC Process Development Lab

As the microelectronics industry continues to change, we have the knowledge and facilities to meet your needs through our dedicated R&D and production sites. Along with these resources and our strong collaborations with key researchers in the field, Sigma-Aldrich continues to develop new products for micro and nanofabrication. We can provide these products with the highest purities (5N, 6N, 7N and higher) up to multi-kilogram scales. We back up our quality with a full range of analytical tests such as ICP-MS. Our volatile precursor products are packaged to specification using our state-of-the-art liquid filling station, to ensure you get what you order every time. Need custom packaging? We have a variety of custom packaging options as shown on pages 10 and 11.



Liquid filling station

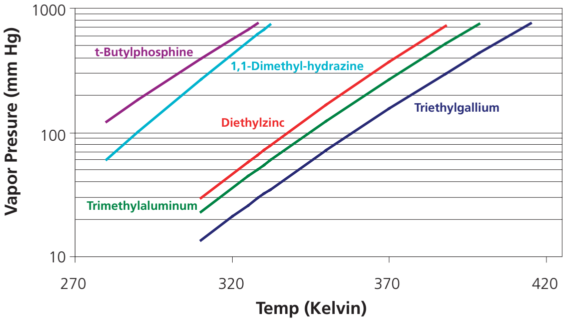
Sheboygan, WI Manufacturing

Analytical Capabilities for Volatile Precursors

ALD and MOCVD processes require key volatility, decomposition, product quality and safety and handling data. Sigma-Aldrich can provide the data you need to make the best choice of precursor including:

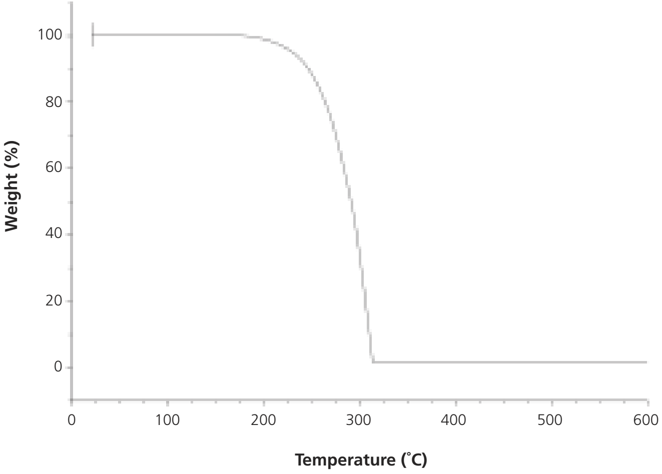
- Vapor Pressure Equation or Graph
- DSC and TGA for decomposition/thermal properties
- ICP-MS for ultra trace elements
- MSDS on all products for safety and handling

Vapor Pressures of Volatile Organometallic Precursors



For product data send an inquiry to **matsci@sial.com**; for MSDS and safety go to the website **www.sigma-aldrich.com** and search by product number.

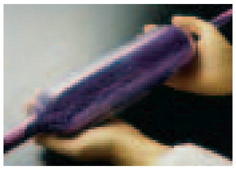
TGA Profile of J1,0000-9
(*N,N'*-Diisopropylacetamidinato)copper(I)



Courtesy of Roy Gordon at Harvard University.

Ready to scale up? For competitive quotes on larger quantities or custom synthesis, contact Sigma-Aldrich Fine Chemicals at 1-800-336-9719 (USA), or visit www.sigma-aldrich.com/safc.

High Purity Inorganics



Aldrich-APL (AAPL) offers a complete line of the highest purity inorganic salts and materials for the micro and nanoelectronics market. Through proprietary processes, AAPL manufactures metal halide salts as anhydrous beads or powders. These ultra-high purity materials have total metals impurities 4N-5N or higher and water contents less than 100 ppm. AAPL can bring its expertise in reactive gas processing, high-temperature synthesis and metal distillations to meet your materials demands. AAPL products are carefully packaged under moisture and air-free conditions, ensuring the quality you expect. Whatever your scale, your demands can be met. If you are looking for a special material and cannot find it here, contact us at **matsci@sial.com**.

Gallium trichloride (beads)

42,712-8
Purity: 99.999+%
CAS No. 13450-90-3
MF: $GaCl_3$
FW: 176.08
Density: 2.47 g/mL

Also available as powder or slugs.
Call for your product configuration

Typical ICP–MS Results for 42,712-8 in ppm

Ag	>0.04	Eu	>0.04	Na	<0.04	Sm	<0.04
Al	<0.04	Fe	0.58	Nb	<0.04	Sn	<0.04
As	<0.04	Ga	Major	Nd	<0.04	Sr	<0.04
Au	<0.04	Gd	<0.04	Ni	0.15	Ta	<0.04
B	0.17	Ge	<0.04	Os	<0.04	Tb	<0.04
Ba	0.18	Hf	<0.04	Pb	<0.04	Te	<0.04
Be	<0.04	Hg	<0.04	Pd	<0.04	Th	<0.04
Bi	<0.04	Ho	<0.04	Pr	0.16	Ti	<0.04
Ca	1.42	In	<0.04	Pt	<0.04	Tl	<0.04
Cd	<0.04	Ir	<0.04	Rb	<0.04	Tm	<0.04
Ce	0.25	K	1.12	Re	<0.04	U	<0.04
Co	<0.04	La	<0.04	Rh	<0.04	V	<0.04
Cr	<0.04	Li	<0.04	Ru	<0.04	W	<0.04
Cs	<0.04	Lu	<0.04	Sb	<0.04	Y	<0.04
Cu	<0.04	Mg	<0.04	Sc	<0.04	Yb	<0.04
Dy	<0.04	Mn	<0.04	Se	<0.04	Zn	<0.04
Er	<0.04	Mo	<0.04	Si	3.72	Zr	<0.04

Hafnium(IV) chloride

59,059-2
Purity: 99.9%
CAS No. 13499-05-3
MF: $HfCl_4$
FW: 320.30

Aluminum trichloride (powder)

56,391-9
Purity: 99.999%
CAS No. 7446-70-0
MF: $AlCl_3$
FW: 133.34
Sublimes at 181 °C

Typical ICP–MS Results for 56,391-9 in ppm

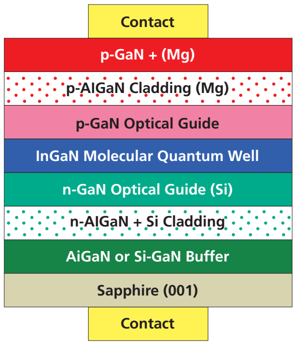
Ag	<0.04	Eu	0.07	Na	1.55	Sm	0.7
Al	<0.04	Fe	0.38	Nb	<0.04	Sn	<0.04
As	<0.04	Ga	1.01	Nd	<0.04	Sr	<0.04
Au	<0.04	Gd	<0.04	Ni	0.13	Ta	<0.04
B	0.23	Ge	<0.04	Os	<0.04	Tb	<0.04
Ba	<0.04	Hf	0.08	Pb	0.5	Te	0.05
Be	<0.04	Hg	<0.04	Pd	<0.04	Th	<0.04
Bi	<0.04	Ho	<0.04	Pr	<0.04	Ti	0.2
Ca	1.03	In	<0.04	Pt	0.05	Tl	<0.04
Cd	<0.04	Ir	<0.04	Rb	<0.04	Tm	<0.04
Ce	<0.04	K	<0.04	Re	<0.04	U	<0.04
Co	<0.04	La	<0.04	Rh	<0.04	V	<0.04
Cr	.023	Li	<0.04	Ru	<0.04	W	<0.04
Cs	0.05	Lu	<0.04	Sb	<0.04	Y	<0.04
Cu	0.12	Mg	1.29	Sc	<0.04	Yb	<0.04
Dy	<0.04	Mn	<0.04	Se	0.11	Zn	1.05
Er	<0.04	Mo	<0.04	Si	1.07	Zr	<0.04

Catalog #	Name	Formula	Metals Purity %	mp °C	bp °C/mmHg*	Sublime °C
44,960-1	Aluminum tribromide	$AlBr_3$	99.999	97.5	263.3/747	
45,086-3	Gallium tribromide	$GaBr_3$	99.999	121.5	279	
42,941-4	Indium trichloride	$InCl_3$	99.999			300
41,365-8	Indium(I) iodide	InI	99.999 beads	351		
57,776-6	Molybdenum hexacarbonyl	$Mo(CO)_6$	99.9		156	
64,245-2	Molybdenum(V) chloride	$MoCl_5$	99.99 powder	194	268	
39,909-4	Molybdenum(VI) fluoride	MoF_5	99.9	17.5	37	
51,069-6	Niobium(V) chloride	$NbCl_5$	99.995	204.7	254	
51,068-8	Tantalum(V) chloride	$TaCl_5$	99.999	216	242	
45,160-6	Titanium(IV) bromide	$TiBr_4$	99.99	39	230	
25,431-2	Titanium(IV) chloride	$TiCl_4$	99.995	-24	136.4	
39,910-8	Tungsten(VI) fluoride	WF_6	99.9	2.3	17.5	
47,295-6	Tungsten hexacarbonyl	$W(CO)_6$	99.9	150		
64,516-8	Tungsten(VI) chloride	WCl_6	99.99 powder	275	346.7	
40,056-4	Zirconium(IV) bromide	$ZrBr_4$	98.0			357
64,764-0	Zirconium(IV) chloride	$ZrCl_4$	99.99			331

**@760 mmHg unless otherwise stated.*

TO ORDER: Contact your local Sigma-Aldrich office (see back cover), call 1-800-558-9160 (USA), or visit sigma-aldrich.com.

III-V Material Sources

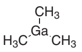


At the forefront of optoelectronic, lighting and data storage applications, III-V semiconductor materials continue to generate exciting new applications. III-V quantum dot heterostructures can address the technical challenges of data transfer and storage issues in telecom and datacom systems. Blue laser GaN LEDs are expected to make a significant impact on HD-DVD storage in the coming years.[10] The figure shows the necessary material layers to construct the blue-violet lasers.[11] GaAs and InP are primary components of low noise and power amplifiers. High brightness LEDs for mobile phones and automotive display lighting are made from a variety of III-V semiconductors. Sigma-Aldrich can provide the highest quality III-V precursors for research and production applications. For aluminum precursors see page 2.

Gallium Precursors

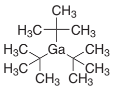
Trimethylgallium

J1,0001-5
CAS No. 1445-79-0
FW: 114.83
mp: -15.8 °C
bp: 55.7 °C
Density: 1.10 g/mL



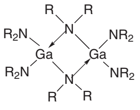
Tri-*tert*-butylgallium

J1,0003-4
CAS No. 55681-99-7
FW: 241.07
bp: 72 °C @ 60 mmHg



Tris(dimethylamido)gallium

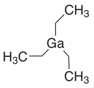
54,653-4
Purity: 98%
CAS No. 57731-40-5
FW: 403.90
mp: 104–105.5 °C



R = CH_3

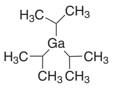
Triethylgallium

J1,0001-7
CAS No. 1115-99-7
FW: 156.91
mp: -82 °C
bp: 109 °C @ 300 mmHg



Triisopropylgallium

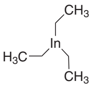
J1,0001-6
CAS No. 54514-59-9
FW: 198.99
bp: 95-98 °C @ 60 mmHg



Indium Precursors

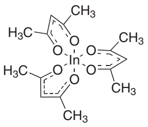
Triethylindium

57,091-5
CAS No. 923-34-2
FW: 202.00
mp: -32 °C
bp: 184 °C
Density: 1.260 g/mL



Indium Acetylacetonate

I,330-0
Purity: 99.99%
CAS No. 14405-45-9
FW: 412.15
mp: 187-189 °C



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III-V Material Sources*—cont'd*

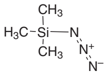
N Sources

Ammonia

29,499-3
Purity: 99.99%
CAS No. 7664-41-7
MF: NH_3
FW: 17.03
mp: -78 °C
bp: -33 °C
Density: 0.6 g/mL

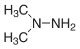
Azidotrimethylsilane

15,507-1
Purity: 95%
CAS No. 4648-54-8
FW: 115.21
bp: 52-53 °C @ 175 mmHg
Density: 0.868 g/mL



N,N-dimethylhydrazine

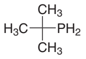
40,680-F
CAS No. 57-14-7
FW: 60.10
bp: 60–62 °C
Density: 0.791 g/mL



P,As and Sb Sources

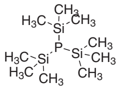
tert-Butylphosphine

49,547-6
Purity: 99.999%
CAS No. 2501-94-2
FW: 90.11
bp: 54–55 °C
Density: 0.738g/mL



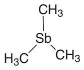
Tris(trimethylsilyl)phosphine

33,367-0
Purity: 95%
CAS No. 15573-38-3
FW: 250.55
bp: 243-244 °C
Density: 0.863 g/mL



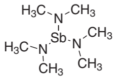
Trimethyl Antimony

J1,0003-3
CAS No. 594-10-5
FW: 166.86



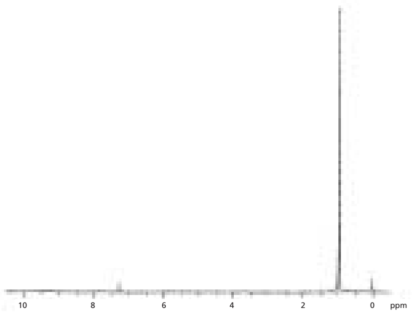
Tris(dimethylamido)antimony

55,397-2
Purity: 99.99%
CAS No. 7289-92-1
FW: 253.98
bp: 32-34 °C @ 0.45 mmHg
Density: 1.325 g/mL



Trimethylarsine

55,131-7
Purity: 99.999%
CAS No. 593-88-4
MF: $(CH_3)_3As$
FW: 120.03
bp: 51 °C
Density: 1.133 g/mL
Chloride: <100ppm



Typical ^{1}H NMR

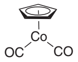
Typical ICP-MS Results for 55,131-7 in ppb

Ag	<1	Fe	<1	Nb	<1	Sm	<1
Al	1	Ga	<1	Nd	<1	Sn	<1
Au	3	Gd	<1	Ni	<1	Sr	<1
B	2	Ge	<1	Os	<1	Ta	<1
Ba	<1	Hf	<1	P	<1	Tb	<1
Be	<1	Hg	<1	Pb	<1	Te	<1
Bi	<1	Ho	<1	Pd	<1	Th	<1
Ca	<1	In	<1	Pr	<1	Ti	<1
Cd	<1	Ir	<1	Pt	<1	Tl	<1
Ce	<1	K	<1	Rb	<1	Tm	<1
Co	<1	La	<1	Re	<1	U	<1
Cr	<1	Li	<1	Rh	<1	V	<1
Cs	<1	Lu	<1	Ru	<1	W	<1
Cu	4	Mg	<1	Sb	3	Y	<1
Dy	<1	Mn	<1	Sc	<1	Yb	<1
Er	<1	Mo	<1	Se	<1	Zn	1
Eu	<1	Na	2	Si	<1	Zr	<1

Precursors for Metallization and Barrier Materials*

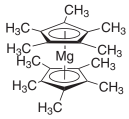
Dicarbonyl(cyclopentadienyl)cobalt(I)

24,525-9
CAS No. 12078-25-0
FW: 180.05
bp: 139–140 °C @ 710 mmHg



Bis(pentamethylcyclopentadienyl)magnesium

51,254-0
Purity: 99.999
CAS No. 74507-64-5
FW: 294.77
mp: 230 °C (D)

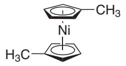


Niobium(V) ethoxide

J1,0003-6
Purity: 99.999%
CAS No. 3236-82-6
MF: $(C_2H_5O)_5Nb$
FW: 318.21

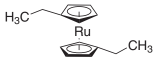
Bis(methylcyclopentadienyl)nickel(II)

51,047-5
Purity: 97%
CAS No. 1293-95-4
FW: 216.96
mp: 34–36 °C
bp: 85–90 °C @ 1 mmHg



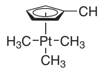
Bis(ethylcyclopentadienyl)ruthenium(II)

64,866-3
CAS No. 32992-96-4
FW: 235.29
mp: 6 °C
bp: 100 °C @ 0.01 mmHg



Cyclopentadienyl(trimethyl)platium(IV)

64,560-5
CAS No. 94442-22-5
FW: 319.31
mp: 30–31 °C

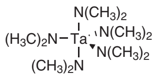


Tantalum(V) ethoxide

51,855-7
Purity: 99.999%
CAS No. 6074-84-6
MF: $(C_2H_5O)_5Ta$
FW: 406.26
mp: 21 °C
bp:155 °C @ 0.01 mmHg
Density: 1.566 g/mL

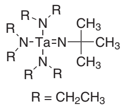
Pentakis(dimethylamido)tantalum(V)

49,686-3
Purity: 99.99%
CAS No. 19824-59-0
FW: 401.33
mp: 100 °C (D)
Density: 1.252 g/mL



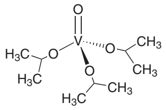
Tris(diethylamido)(tert-butylimido)tantalum(V)

52,128-0
Purity: 99.99%
CAS No. 169896-41-7
FW: 468.46
Density: 1.252 g/mL



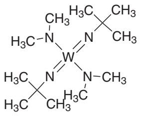
Vanadium(V) oxytriisopropoxide

40,492-6
CAS No. 5588-84-1
FW: 244.21
bp: 80–82 °C @ 2 mmHg



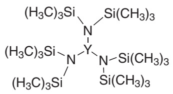
Bis(*tert*-butylimido)bis(dimethylamido)tungsten(VI)

57,793-6
CAS No. 406462-43-9
MF: $C_{12}H_{30}N_4W$
FW: 414.23



Tris(*N*,*N*-bis(trimethylsilyl)amide)yttrium(III)

52,451-4
CAS No. 41836-28-6
FW: 570.07
mp: 161–166 °C



Yttrium(III) butoxide solution 0.5M in toluene

51,066-1
CAS No. 111941-71-0
MF: $(C_4H_9O)_3Y$
FW: 308.25
bp: 109 °C

Diethylzinc

25,678-1
CAS No. 557-20-0
MF: $(C_2H_5)_2Zn$
FW: 123.49
mp: -28 °C
bp: 117 °C
Density: 1.205 g/mL

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*For titanium precursors see page 3.

High Purity Deposition Gases

High Purity CVD Gases are used in the deposition of amorphous and epitaxial silicon, SiGe alloys, and dielectrics as well as the manufacture of integrated circuits and photovolatics. The gases are also used as dopants in CVD and ion-implantation processes. Deuterated gases have been shown to improve device performance and reliability. ISOTEC™, a key member of the Sigma-Aldrich family, produces our stable isotope product lines. Led by an impressive group of expert scientists, ISOTEC™ routinely engages in multiple step syntheses of complex labeled molecules including the stable isotope labeling patterns ^{13}C, ^{15}N, ^{17}O, ^{18}O, ^{2}H. ISOTEC™ has a large inventory of stable isotope labeled starting material to accommodate any researcher's need. Contact ISOTEC™ at **www.sigma-aldrich.com/isotec**.

Catalog Number	Product Name	Formula	Purity (%)	bp °C	Vapor density (vs. Air)	Critical Temp °C	Water	H_2	N_2	O_2	CH_4	Other
							(ppm)					
46,305-1	Diborane (10% in H_2)	B_2H_6	99.99*	-92.5	–	–	–	–	–	–	–	
46,313-2	Diborane-d_6 (10% in D_2)	B_2D_6	99.99*	-92.5	–	–	–	–	–	–	–	
46,314-0	Diborane-d_6 (10% in He)	B_2D_6	99.99*	-92.5	–	–	–	–	–	–	–	
46,307-8	Digermane (10% in H_2)	Ge_2H_6	99.99	31.5	–	150.9	–	–	–	–	–	
46,304-3	Disilane	Si_2H_6	99.998	-14.5	–	150.9	<1	–	<1	<1	–	<50 higher silanes
46,302-7	Germane	GeH_4	99.997	-88.4	1.53 (-142 °C)	35	<1	<50	<2	<0.5	–	<20 digermane
46,299-3	Methylsilane	CH_3SiH_3	99.9	-57	0.628 (-58 °C)		–	–	<10	<2	<50	<100 higher silanes
29,564-7	Phosphine	PH_3	99.9995	-87.5	1.15	51.3	<1	–	<1	<1	<1	<1 AsH_3
46,312-4	Phosphine-d_3	PD_3	98 atom %	-87.5	–	–		–	–	–	–	
33,389-1	Silane	SiH_4	99.998	-112	1.1	-3.4	<1	<100	<2	–	–	<5 higher silanes
46,311-6	Silane-d_4	SiD_4	98 atom%	-112	–	–	–	–	–	–		
39,635-4	Tetramethyl-germanium	$(CH_3)_4Ge$	98%	43.5	0.978	–	–	–	–	–	–	
46,309-4	Trimethylboron	$(CH_3)_3B$	98.35	-20.2	2.3	–	–	<50	<10	<1	<100	<1000 N $(CH_3)_3$
46,342-6	Trimethylboron-d_9	$(CD_3)_3B$	99 atom %	-20.2	2.3	–	–	–	–	–		

*As diborane

Custom Packaging

Sigma-Aldrich has a variety of packaging options to ensure the quality and safe handling of all of our volatile precursors. Most of our products come in standard packaging depending on size, quantity and material state. Custom packing is optional for all of our products. If a product catalog number starts with a "J", then packaging configuration is up to you at the time you order.

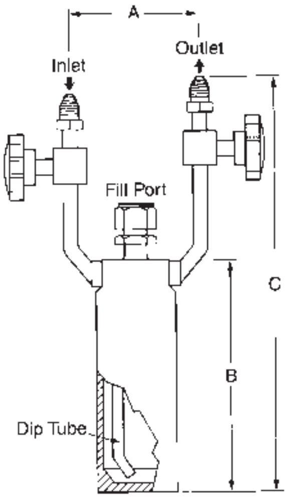
Borosilcate or Quartz Ampules	For handling small quantities in a dry-box. Shipped in a clam-shell.
Sure/Seal™ Bottles	The standard container for air sensitive materials.
Gas Lecture Bottles	Electronic grade gases packed in clean room conditions.
Sure/Pac™ Cylinder	Equipped with brass ball valve and treated plug.
Stainless Steel Bubblers	Standard and custom sizes for your deposition systems.

Stainless Steel Bubblers

For Deposition Precursors

Sigma-Aldrich offers stainless steel bubblers designed to deliver our ultra high-purity organometallic precursors to the reaction zone during the fabrication process. All of our volatile precursors can be prepackaged in these bubblers to ensure you are getting the highest quality material available.

In addition to our standard sizes, Sigma-Aldrich can custom build bubblers to your equipment specifications. Please inquire about custom bubbler configurations by using the drawing below, calculate your dimensions then contact Sigma-Aldrich at **matsci@sial.com**.



Stock Stainless Steel Bubblers

- Vertical, dual-valve bubblers equipped with a $^1/_2$ in. fill port and $^1/_4$ in. VCR™ inlet and outlet valves.
- Electropolished 316L stainless steel that is free of mechanical defects and foreign chemical contaminants.
- Sealed in a clean-room environment to ensure product quality and integrity.
- Pneumatically tested to ensure leak-free service.
- Available from stock in the sizes listed below.

Size	Dimensions (A x B x C) in.	Cat. No.
300 mL	3.25 x 7.36 x 12.81	**Z52,706-8**
1.2 L	2.77 x 8.00 x 10.28	**Z55,336-0**

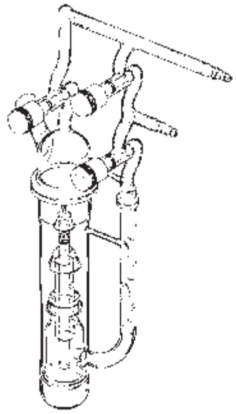
Custom Stainless Steel Bubblers

- Full range of sizes available.
- Specify the dimensional requirements (A, B, C) as shown in the diagram.
- Select inlet and outlet valve connections.

VCR is a trademark of Swagelok Co.

Aldrich 3-Stage Oil Diffusion Pump

Aldrich 3-stage oil diffusion pumps provide fast 375 L/s pumping speed that outperforms traditional glass diffusion pumps. They feature all glass construction with a removable jet assembly for easy cleaning. 3-stage oil diffusion pumps safely reduce sublimation and distill action temperature and are chemically resistant to acidic solvents. Sigma-Aldrich also offers all the necessary equipment to run and maintain your pump.



Model	Overall dim. (in.)	Pumping speed (L/s)	Max. vacuum (torr)	Catalog Number
With Gauge Port	32 x 12	375	10	**Z54,478-7**
Without Gauge Port	32 x 12	375	10	**Z55,537-1**

Equipment Required for Diffusion Pump Operation

Description		
Dow Corning Diffusion Pump Oil (500 mL)	Type 704* **44,597-5**	Type 705** **44,598-3**
Leybold Trivac B, D8B Mechanical Vac. Pump, 197 Lpm speed	115 V **Z28,459-9**	220 V **Z28,282-0**
Glas-Col 500 mL Heating Mantle For heating mantle	115 V **Z28,485-8**	230 V **Z28,514-5**
Digitrol II Heat Controller	115 V **Z28,549-8**	240 V **Z28,550-1**
Corning 5x7" Stir Plate	115 V **Z26,206-4**	230 V **Z26,207-2**
Dewar flask, 10 L capacity	**Z10,565-1**	
Safety shield	**Z23,140-1**	
Vacuum Trap 1 L bulb capacity	**F 9776**	

*For Pressures 10^{-5} to 10^{-6} torr **For Pressures 10^{-9} to 10^{-10} torr

Deposition Substrates and Silicon Wafers

Successful deposition of materials often depends on the proper substrates, with a good lattice match and a clean, even surface. Aldrich is proud to offer a variety of new single crystal substrates and silicon wafers in multiple orientations to meet your deposition needs. All these materials undergo rigorous analytical testing including trace metal analysis and x-ray diffraction in order to insure the highest purity standards. If there is an orientation or material you cannot find please contact us at **matsci@sial.com**.

Single Crystal Substrates (10 x 10 x 0.5 mm, single side polished)

Composition	Formula	mp (°C)	Unit Cell (Å)	Orientation							
				Hex (0001)	Cubic (100)	Cubic (110)	Cubic (111)	Rhomb (100)[1]	Tetrag (100)	Tetrag (001)	Tetrag (110)
Aluminum oxide	Al_2O_3	2040	a=4.758 c=12.992	**63,487-5**	–	–	–	–	–	–	–
Lanthanum aluminum oxide	$LaAlO_3$	2080	a=5.357 c=13.22	–	–	–	–	**63,473-5**	–	–	–
LSAT Lanthanum aluminum oxide-strontium aluminum tantalum oxide	$(LaAlO_3)_{0.3}$ $(Sr_2AlTaO_6)_{0.7}$	1840	a=3.868	–	**63,505-0**	–	–	–	–	–	–
Magnesium aluminate	$MgAl_2O_4$	2130	a=8.083	–	**63,507-3**	**63,484-0**	**63,483-2**	–	–	–	–
Magnesium oxide	MgO	2852	a=4.216	–	**63,464-6**	**63,470-0**	**63,469-7**	–	–	–	–
Silicon dioxide, optical grade	SiO_2	1610	a=4.914 c=5.405	**63,486-7**	–	–	–	–	–	–	–
Strontium lanthanum aluminate	$SrLaAlO_4$	1650	a=3.756 c=12.63	–	–	–	–	–	**63,511-1**	**63,489-1**	–
Strontium titanate	$SrTiO_3$	2080	a=3.905	–	**63,468-9**	**63,467-0**	**63,816-1**	–	–	–	–
Titanium(IV) oxide rutile	TiO_2	1840	a=4.5936 c=2.9582	–	–	–	–	–	**63,504-9**	**63,505-7**	**63,506-5**
Yttrium vanadate	YVO_4	1825	a=7.12 c=6.29	–	–	–	–	–	–	–	**63,510-3**

1) Cubic @>435 °C, a=3.821 Å

Silicon Wafers (0.5 mm thick, single side polished)

Catalog Number	Orientation	Radius (in.)	Semiconductor Type	Dopant	Resistivity (Ω cm)
64,668-7	(100)	2	–	none	10^2–10^4
64,710-1	(111)	2	–	none	10^2–10^4
64,753-5	(100)	3	–	none	10^2–10^4
64,754-3	(111)	3	–	none	10^2–10^4
64,767-5	(100)	2	P-type	boron	10^{-3}–40
64,770-5	(111)	2	P-type	boron	10^{-3}–40
64,776-4	(100)	3	P-type	boron	10^{-3}–40
64,777-2	(111)	3	P-type	boron	10^{-3}–40
64,778-0	(100)	2	N-type	phosphorous	10^{-3}–40
64,779-9	(111)	2	N-type	phosphorous	10^{-3}–40
64,780-2	(100)	3	N-type	phosphorous	10^{-3}–40
64,781-0	(111)	3	N-type	phosphorous	10^{-3}–40

Silicon wafers have a density of 2.33 g/mL; unit cell: cubic, a = 5.4037 Å

Gold-Coated Substrates

We now offer gold-coated substrates with 100 to 2000 Å gold coatings on: Glass microscope slides, round and square coverslips, silicon wafers, or mica. Please visit us at **www.sigma-aldrich.com** for more information.

Books and Software

CVD of Nonmetals

Z28,630-3

W.S. Rees, Jr., Ed., John Wiley & Sons, 1992, pp. 392, Hardcover.

The basics necessary for any CVD process are discussed. Precursor requirements, with an emphasis on materials chemistry, common structures of reactants and substrates, as well as reaction control are discussed for a broad range of compositions. Technological issues, such as reactor geometries and operation parameters, are assessed and the viability of the method is compared with other techniques for the preparation of thin films.

Inorganic Materials

Z40,867-0

D.W. Bruce and D. O'Hare, Eds., John Wiley & Sons, 1997, pp. 607, Softcover.

This new edition of the acclaimed Inorganic Materials reflects the expansion in both knowledge and interest that materials chemistry has experienced in recent years. It provides a well-referenced introduction to the most exciting aspects of materials chemistry, followed by an overview with examples chosen to best emphasize the materials in question.

Characterization of Materials, 2 volume set

Z55,373-5

Elton N. Kaufmann, John Wiley & Sons, 2003, pp. 1392, Hardcover.

Provides comprehensive coverage of materials characterization techniques including computational and theoretical methods, crystallography, mechanical testing, thermal analysis, optical imaging and spectroscopy.

Molecular Nanoelectronics

Z55,011-6

Mark Reed and Tahkee Lee, American Scientific Publishers, 2003, pp. 400, Hardcover.

This book covers topics on transport theory through nanostructures, processing, self-assembly, device fabrication and architecture for nanoelectronic device applications. Contains about 2,000 bibliographic citations and hundreds of illustrations, figures, tables, chemical structures and equations.

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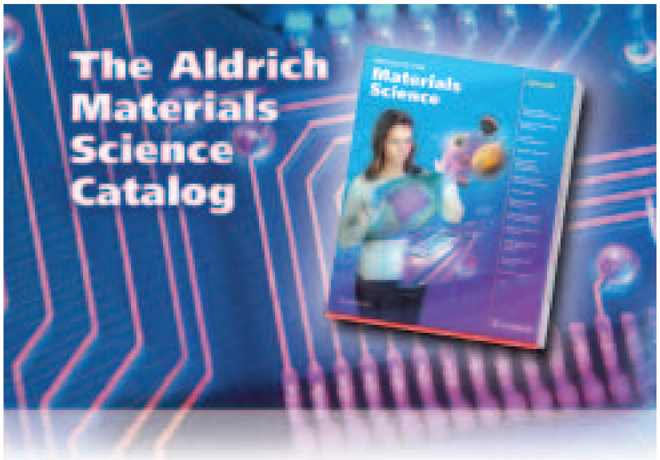

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