

Material Matters™

Vol. 2 Supplement, 2007



New Products 2007



*Our Chemistry Driving
Your Performance.*

- Biomaterials
- Energy Storage
- Thin Film Deposition
- Metals and Ceramics
- Nanomaterials
- Organic Electronics and Photonics
- Self-Assembly

Introduction

Material Matters[™] is gaining wide acceptance as a technical periodical, evidenced by the frequency and quality of citations. Well-received by fellow scientists, each issue focuses on a single theme and offers concise technical reviews by leading experts. Sigma-Aldrich Materials Science products related to the issue topics are also included. Regular readers of *Material Matters* may notice the addition of "Your Materials Matter," a feature highlighting topics and materials that were specifically requested by researchers.

In contrast to the regular issues of *Material Matters*, this supplement is a selection of over 100 of the latest new products from Sigma-Aldrich Materials Science. These products have been developed through our Materials Chemistry Centers of Excellence in research and manufacturing and through collaborative partnerships. The materials have been organized by "research interest" categories including biomaterials, energy storage, thin film deposition, metals & ceramics, nanomaterials, organic electronics and photonics, and molecular self-assembly.

For the most up-to-date list of Materials Science & Engineering research products, please visit our Web site:

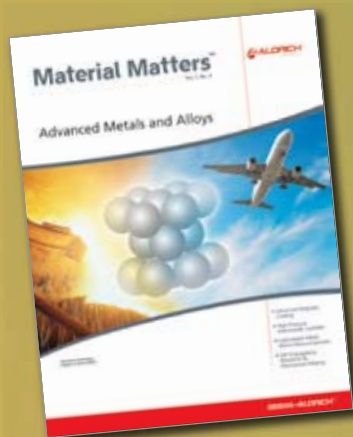
sigma-aldrich.com/msnew

As you continue to explore the frontiers of materials science and engineering, we hope that this supplement and our comprehensive Materials Chemistry offering further drive your research performance. We strive to provide innovative materials that meet your R&D needs. Your materials matter. Tell us what materials will accelerate your research, and we will carefully consider adding them to our portfolio of products. Please send your suggestions to matsci@sial.com—your suggestion could be the topic of the "Your Materials Matter" feature in the *Material Matters* periodical!

Shashi Jasty, Ph.D.
Materials Science
Sigma-Aldrich Corporation

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What Matters in Materials Research? Material Matters[™]



A Technical Periodical from Sigma-Aldrich Materials Science

Hot Topics Expert Reviews

Recent Thematic Issues featured:

- Polymerization
- Self-Assembly
- Thin Film Deposition
- Nanomaterials Applications
- Hydrogen Storage
- Organic Electronics

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Biomaterials

For a complete list of biocompatible and biodegradable materials, please visit us at sigma-aldrich.com/biomaterials.

3-(Acetylthio)propionic acid, 96%

S-Acetyl-3-mercaptopropionic acid

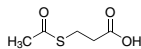
$C_5H_8O_3S$

FW 148.18

[41345-70-4]

mp 48 to 52 °C

687081-5G 5 g



Poly(styrene)-block-poly(ethylene glycol)

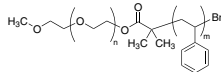
Polystyrene-polyethylene glycol polymersome forming polymer

M_n 800-1200 (PEG)

M_n 22,500-27,500

M_n 20,700-25,300 (polystyrene)

686476-500MG 500 mg



Poly(styrene)-block-poly(acrylic acid)

Polystyrene-polyacrylic acid polymersome forming polymer

M_n 1890-2310 (poly(acrylic acid))

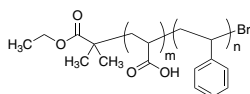
M_n 7470-9130

M_n 5580-6820 (polystyrene)

solubility

tetrahydrofuransoluble

686794-500MG 500 mg



Poly(ethylene glycol)dimethacrylate

[25852-47-5]

bp..... >200 °C/2 mm Hg

► average M_n ~6000

T_m 50.2 to 53.7 °C

687537-1G 1 g

► M_n ~2000

687529-1G 1 g

Glycolide, >99%

1,4-Dioxane-2,5-dione

$C_4H_4O_4$

FW 116.07

[502-97-6]

mp 82 to 86

G1796-25G 25 g



Energy Storage Materials

For a complete list of materials for energy storage applications, please visit us at sigma-aldrich.com/hydrogen.

Metal Alloys

Reference kit for hydrogen storage

Components

Lanthanum nickel alloy, $LaNi_5$ (Aldrich 685933) 10g

Lanthanum nickel alloy, $LaNi_{4.5}Co_{0.5}$ (Aldrich 685968) 10g

Mischmetal nickel alloy (Aldrich 685976) 10g

Titanium manganese alloy (Aldrich 685941) 10g

686115-1KT 1 kit

Lanthanum nickel alloy, $LaNi_5$

Lanthanum pentanickel

$LaNi_5$

FW 432.37

► hydrogen-storage grade

685933-10G 10 g

Lanthanum nickel alloy, $LaNi_{4.5}Co_{0.5}$

$LaNi_{4.5}Co_{0.5}$

FW 432.49

[130469-99-7]

685968-10G 10 g

Mischmetal nickel alloy

(Ce, La, Nd, Pr) Ni_5

[54426-34-5]

685976-10G 10 g

Titanium manganese alloy

$TiMn_2$ type, Laves phase

[220316-38-1]

► $TiMn_2$, alloy 5800, hydrogen-storage grade

685941-10G 10 g

Hydrides & Amides

Hydrogen Storage Materials for Research, Kit

Components

Lithium amide (Aldrich 686050) 10g
 Sodium amide (Aldrich 686042) 10g
 Lithium nitride (Aldrich 399558) 10g
 Lithium aluminum hydride (Aldrich 686034) 10g
 Sodium aluminum hydride (Aldrich 685984) 10g
 Lithium hydride (Aldrich 201049) 10g
 Sodium hydride (Aldrich 223441) 10g
 Lithium borohydride (Aldrich 686026) 10g
 Sodium borohydride (Aldrich 686018) 10g
 Magnesium hydride (Aldrich 683043) 10g

686093-1KT 1 kit

Borane-ammonia complex

H₆BN H₃N-BH₃
 FW 30.87
 [13774-81-7]

▶ 97%

682098-1G 1 g
 682098-10G 10 g

▶ 90%, technical grade

287717-1G 1 g
 287717-10G 10 g

Calcium hydride, 95%

H₂Ca CaH₂
 FW 42.09
 [7789-78-8]
 EC No. 2321892

▶ reagent grade, lumps, +4 mesh

mp..... 190 °C
 213322-10G 10 g
 213322-100G 100 g
 213322-500G 500 g

Hexadecahydropyrene, 95%

C₁₆H₂₆
 FW 218.38
 [2435-85-0]



density..... 0.984 g/mL, 25 °C
 n_D²⁰..... 1.521
 691704-1G 1 g

Lithium aluminum hydride

H₄AlLi LiAlH₄
 FW 37.95
 [16853-85-3]
 EC No. 2408779

▶ hydrogen-storage grade

mp..... 125 °C (dec.)
 686034-10G 10 g

Lithium amide

H₂LiN LiNH₂
 FW 22.96
 [7782-89-0]
 EC No. 2319684

▶ hydrogen-storage grade

mp..... 380 to 400 °C
 density..... 1.178 g/mL, 25 °C
 686050-10G 10 g

Lithium borohydride, 90+%

H₄BLi LiBH₄
 FW 21.78
 [16949-15-8]
 EC No. 2410217

▶ hydrogen-storage grade

mp..... 275 °C (dec.)
 density..... 0.666 g/mL, 25 °C
 686026-10G 10 g

Lithium hydride, 95%

HLi LiH
 FW 7.95
 [7580-67-8]
 EC No. 2314843

▶ powder, -30 mesh

mp..... 680 °C
 density..... 0.82 g/mL, 25 °C
 201049-5G 5 g
 201049-10G 10 g
 201049-100G 100 g
 201049-500G 500 g

Lithium nitride

Li₃N
 FW 34.83
 [26134-62-3]

▶ -80 mesh

mp..... 840 to 850 °C (N₂)
 density..... 1.3 g/mL, 25 °C
 399558-5G 5 g
 399558-10G 10 g
 399558-25G 25 g

Sodium amide

H₂NNa NH₂Na
 FW 39.01
 [7782-92-5]
 EC No. 2319710

▶ hydrogen-storage grade

bp..... 400 °C
 mp..... 210 °C
 686042-10G 10 g

Sodium borohydride, 98%

Sodium tetrahydridoborate NaBH₄
 H₄BNa
 FW 37.83
 [16940-66-2]
 EC No. 2410044

▶ hydrogen-storage grade

mp..... >300 °C (dec.)
 686018-10G 10 g

Sodium hydride, 95%

HNa NaH
 FW 24.00
 [7646-69-7]
 EC No. 2315873

▶ dry

mp..... 800 °C (dec.)
 223441-10G 10 g
 223441-50G 50 g
 223441-250G 250 g
 223441-1KG 1 kg

TO ORDER: Contact your local Sigma-Aldrich office (see back cover),
 or visit sigma-aldrich.com/matsci.

Catalysts

Catalysts for Hydrogen Storage Research, Kit

Components

Niobium(V) oxide (Aldrich 208515) 1g
 Titanium(III) chloride (Aldrich 686085) 1g
 Titanium(II) hydride (Aldrich 686069) 1g
 Zirconium(II) hydride (Aldrich 208558) 1g
 Vanadium(III) chloride (Aldrich 208272) 1g
 Scandium(III) chloride (Aldrich 686077) 1g

686107-1KT 1 kit

Niobium(V) oxide, 99.9%

Niobium pentoxide Nb₂O₅
 FW 265.81
 [1313-96-8]
 EC No. 2152136

► -325 mesh

density.....4.47 g/mL, 25 °C
 208515-1G 1 g
 208515-100G 100 g
 208515-500G 500 g

Scandium(III) chloride, 99.9%

Cl₃Sc ScCl₃
 FW 151.31
 [10361-84-9]

► hydrogen-storage grade

mp.....960 °C
 density.....2.39 g/mL, 25 °C
 686077-1G 1 g

Titanium(II) hydride

H₂Ti TiH₂
 FW 49.88
 [7704-98-5]
 EC No. 2317268

► hydrogen-storage grade

mp.....>400 °C (dec.)
 density.....3.91 g/mL, 25 °C
 686069-1G 1 g

Titanium(III) chloride, 99.99+%

Titanium trichloride TiCl₃
 Cl₃Ti
 FW 154.23
 [7705-07-9]
 EC No. 2317289

► hydrogen-storage grade

mp.....440 °C (dec.)
 686085-1G 1 g

Vanadium(III) bromide, 99%

Br₃V VBr₃
 FW 290.65
 [13470-26-3]
 density.....4 g/mL, 25 °C
 691798-1G 1 g

Vanadium(III) chloride, 97%

Cl₃V VCl₃
 FW 157.30
 [7718-98-1]
 EC No. 2317446
 density.....3 g/mL, 25 °C
 208272-1G 1 g
 208272-5G 5 g
 208272-25G 25 g

Zirconium(II) hydride, 99%

H₂Zr ZrH₂
 FW 93.24
 [7704-99-6]
 EC No. 2317273

► -325 mesh

208558-1G 1 g
 208558-100G 100 g

Materials for Thin Film Deposition

For a complete list of materials for thin film deposition applications, please visit us at sigma-aldrich.com/precursors.

ALD Precursors

Silicon tetrachloride

Tetrachlorosilane SiCl₄
 Cl₄Si
 FW 169.90
 [10026-04-7]
 EC No. 2330540

► for Cambridge NanoTech Inc. ALD system

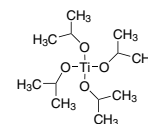
99.998%
 bp.....57.6 °C
 mp.....-70 °C
 density.....1.483 g/mL, 25 °C
 688509-25ML 25 mL

Titanium(IV) isopropoxide

Tetraisopropyl orthotitanate
 C₁₂H₂₈O₄Ti
 FW 284.22
 [546-68-9]
 EC No. 2089096
 BRN 3679474

► for Cambridge NanoTech Inc. ALD system

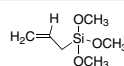
bp.....232 °C
 mp.....14 to 17 °C
 density.....0.96 g/mL, 20 °C
 687502-25G 25 g



Solgel Precursors — Silanes

Allyltrimethoxysilane, 98+%

$C_6H_{14}O_3Si$
FW 162.26
[2551-83-9]
EC No. 2198558
BRN 2350745

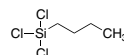


► deposition grade

bp..... 146-148 °C
density..... 0.963 g/mL, 25 °C
679267-50G 50 g

Butyltrichlorosilane, 98+%

$C_4H_9Cl_3Si$
FW 191.56
[7521-80-4]
EC No. 2313813
BRN 1736032

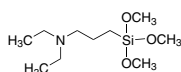


► deposition grade

bp..... 149 °C
density..... 1.16 g/mL, 25 °C
679224-50G 50 g

[3-(Diethylamino)propyl]trimethoxysilane, 98+%

N,N-Diethyl-3-(trimethoxysilyl)propylamine
 $C_{10}H_{25}NO_3Si$
FW 235.40
[41051-80-3]
EC No. 2551920



► deposition grade

bp..... 120 °C/20 mm Hg
density..... 0.95 g/mL, 25 °C
679356-50G 50 g

Ethyltrichlorosilane, ≥98% (GC)

Trichloro(ethyl)silane
 $C_2H_5Cl_3Si$
FW 163.51
[115-21-9]
EC No. 2040726
BRN 1361384

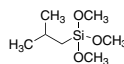


► deposition grade, 99.99+% (as metals)

bp..... 99 °C
mp..... -106 °C
density..... 1.238 g/mL, 25 °C
679216-50G 50 g

Isobutyl(trimethoxy)silane, 98+%

$C_7H_{18}O_3Si$
FW 178.30
[18395-30-7]
EC No. 2422725
BRN 2233976



► deposition grade

bp..... 154 °C
density..... 0.93 g/mL, 25 °C
bp..... 137 °C
679364-50G 50 g

Methyltrichlorosilane, ≥98% (GC)

Trichloro(methyl)silane
 CH_3Cl_3Si
FW 149.48
[75-79-6]
EC No. 2009026
BRN 1361381

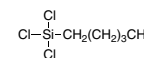


► deposition grade, 99.99+% (as metals)

bp..... 66 °C
density..... 1.273 g/mL, 25 °C
679208-50G 50 g

Pentyltrichlorosilane, 98+%

Amyltrichlorosilane
 $C_5H_{11}Cl_3Si$
FW 205.59
[107-72-2]

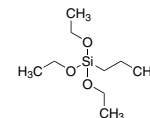


► deposition grade

bp..... 173 °C/760 mm Hg
density..... 1.142 g/mL, 25 °C
679194-50G 50 g

N-Propyltriethoxysilane, 98+%

$C_9H_{22}O_3Si$
FW 206.35
[2550-02-9]

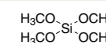


► deposition grade

bp..... 179-180 °C
density..... 0.892 g/mL, 25 °C
679321-50G 50 g

Tetramethyl orthosilicate, 98+%

Tetramethoxysilane
 $C_4H_{12}O_4Si$
FW 152.22
[681-84-5]
EC No. 2116564
BRN 1699658

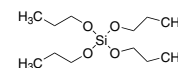


► deposition grade, 99.9+% (metals basis)

bp..... 121-122 °C
mp..... -4 °C
density..... 1.023 g/mL, 25 °C
679259-50G 50 g

Tetrapropyl orthosilicate, 98+%

Tetrapropoxysilane
 $C_{12}H_{28}O_4Si$
FW 264.43
[682-01-9]
EC No. 2116590
BRN 1706115

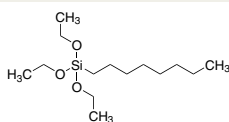


► deposition grade

bp..... 94 °C/5 mm Hg
density..... 0.916 g/mL, 25 °C
679240-50G 50 g

Triethoxy(octyl)silane, ≥98%

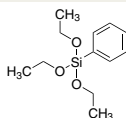
Octyltriethoxysilane
 $C_{14}H_{32}O_3Si$
 FW 276.49
 [2943-75-1]
 EC No. 2209412
 BRN 2325287

▶ **deposition grade, 99.99% (metals basis)**

bp.....84-85 °C/0.5 mm Hg
 density.....0.88 g/mL, 25 °C
 679305-50G 50 g

Triethoxyphenylsilane, 98+%

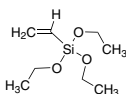
Phenyltriethoxysilane
 $C_{12}H_{20}O_3Si$
 FW 240.37
 [780-69-8]
 EC No. 2123058
 BRN 2940602

▶ **deposition grade**

bp.....112-113 °C/10 mm Hg
 density.....0.996 g/mL, 25 °C
 679291-50G 50 g

Triethoxyvinylsilane, 98+%

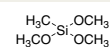
(Triethoxysilyl)ethylene; Vinyltriethoxysilane
 $C_8H_{18}O_3Si$
 FW 190.31
 [78-08-0]
 EC No. 2010817
 BRN 1767229

▶ **deposition grade**

bp.....160-161 °C; 62-63 °C/20 mm Hg
 density.....0.903 g/mL, 25 °C
 679275-50G 50 g

Trimethoxymethylsilane, 98+%

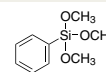
Methyltrimethoxysilane
 $C_4H_{12}O_3Si$
 FW 136.22
 [1185-55-3]
 EC No. 2146850
 BRN 1736151

▶ **deposition grade**

bp.....102-104 °C
 density.....0.955 g/mL, 25 °C
 679232-50G 50 g

Trimethoxyphenylsilane, ≥98%

Phenyltrimethoxysilane; (Trimethoxysilyl)benzene
 $C_9H_{14}O_3Si$
 FW 198.29
 [2996-92-1]
 EC No. 2210669
 BRN 2937896

▶ **deposition grade**

bp.....233 °C
 density.....1.062 g/mL, 25 °C
 679313-50G 50 g

Metals and Ceramics

For a complete list of metal and ceramic materials, please visit us at sigma-aldrich.com/metals.

Gadolinium, 99.99% (REM)

Gd
 FW 157.25
 [7440-54-2]
 EC No. 2311622
 bp.....3273 °C
 resistivity.....126 μΩ-cm, 20°C
 mp.....1313 °C
 density.....7.886 g/mL, 25 °C
 691771-10G 10 g

Iron phosphide, Fe₂P

Ferrous phosphide; Iron diphosphide; Iron phosphide
 Fe_2P
 FW 142.66
 [1310-43-6]
 691658-5G 5 g

Iron phosphide, Fe₃P

Fe_3P
 FW 198.51
 [12023-53-9]
 691593-5G 5 g

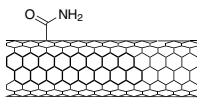


Nanomaterials

For a complete list of nanomaterials, please visit us at sigma-aldrich.com/nano.

Carbon Nanotubes

Carbon nanotube, single-walled, amide functionalized, 80-90% as SWCNT (relative carbonaceous purity)



► diam. 4-6 nm × length 0.7-1.0 μm, bundle dimensions

solubility

DMF	0.5-1.0 mg/mL, with sonication
alcohols	0.5-1.0 mg/mL, with sonication
acetone	0.5-1.0 mg/mL, with sonication
extent of labeling	per 4 atom % (amide groups)
metals	6-8%
685380-100MG	100 mg

Carbon nanotube array, multi-walled

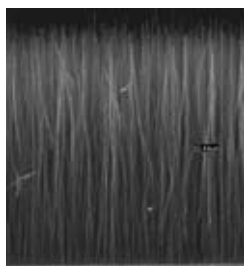
MWCNT array

>99.9% MWCNT

composition

Carbon content >99.9% (structured (sp²) carbon. <0.1% amorphous (sp³) carbon.)

diam. × length..... 100 nm ± 10% × 30 μm ± 10%



CNT Array Side View



CNT Array Package

► vertically aligned on silicon wafer substrate

(1cm X 1cm Si wafer substrate, {100}, 650-1000μm thick, low n-doped (phosphorus), resistivity 1-30 ohm-cm.)

surface coverage (MWCNT) ~2 × 10⁹ CNT/cm² ~20/μm²

687804-1EA 1 ea

► vertically aligned on copper wafer substrate

(1cm X 1cm X 0.05cm high conductivity low-oxygen copper substrate)

surface coverage (MWCNT) ~2 X 10⁹ CNT/cm² ~20/μm²

687812-1EA 1 ea

Nanoclays

Nanoclay, surface modified

Montmorillonite clay

base material Montmorillonite clay

Nanomer® I.28E

► contains 25-30 wt. % trimethyl stearyl ammonium

682608-500G 500 g

Nanomer® I.30E

► contains 25-30 wt. % octadecylamine

682616-500G 500 g

Nanomer® I.44P

► contains 35-45 wt. % dimethyl dialkyl (C14-C18) amine

682624-500G 500 g

Nanomer® I.31PS

► contains 15-35 wt. % octadecylamine, 0.5-5 wt. % aminopropyltriethoxysilane

682632-500G 500 g

Nanomer® I.34TCN

► contains 25-30 wt. % methyl dihydroxyethyl hydrogenated tallow ammonium

682640-500G 500 g

Nanoclay, hydrophilic bentonite

Montmorillonite clay, bentonite; Nanomer® PGV

[1302-78-9]

682659-500G 500 g

Halloysite Nanoclay

Kaolin clay

(Al₂Si₂O₅(OH)₄ · 2 H₂O)

[1332-58-7]

nanopowder

*n*_D²⁰..... 1.54

exchange capacity 8.0

diam. × L..... 30 nm × 0.5-4 μm, nanotube

color 75-96 Hunter Brightness

surface area 64 m²/g

density 2.53 (true specific gravity)

pore volume 0.21-0.34 mL/g



685445-500G 500 g

Nanoparticles

Hydroxyapatite, 97+%

Calcium hydroxyphosphate; HAp
 $[\text{Ca}_5(\text{OH})(\text{PO}_4)_3]_x$
 FW 502.31
 [12167-74-7]

► **nanopowder, particle size <200 nm (BET), 97+%, synthetic**

solid
 mp 1100 °C
 surface area >9.4 m²/g
 677418-5G 5 g
 677418-10G 10 g

Silver

Ag
 FW 107.87

► **nanoparticles, dispersion, particle size ~157 nm, 0.25 mM in H₂O, contains citrate as stabilizer**

n_D^{20} 1.333
 675318-5ML 5 mL

Iron(II,III) oxide solution

Fe₃O₄
 FW 231.53
 [1317-61-9]

► **nanoparticles, dispersion, particle size <150 nm, 10 wt. % in H₂O**

contains ~1% citrate as stabilizer
 679151-10ML 10 mL

Copper, 99.9+%

Cu
 FW 63.55
 [7440-50-8]
 EC No. 2311596

► **nanopowder, particle size <50 nm (TEM)**

bp 2567 °C
 resistivity 1.673 μΩ-cm, 20°C
 mp 1083.4 °C
 684007-25G 25 g

Platinum, 99.9+%

Pt
 FW 195.08
 [7440-06-4]
 EC No. 2311161

► **nanopowder, particle size <50 nm (BET)**

bp 3827 °C
 resistivity 10.6 μΩ-cm, 20°C
 mp 1772 °C
 685453-500MG 500 mg

Palladium, >99.9%

Pd
 FW 106.42
 [7440-05-3]
 EC No. 2311156

► **nanopowder, particle size <25 nm (TEM)**

bp 2970 °C
 resistivity 9.96 μΩ-cm, 20°C
 mp 1554 °C
 686468-500MG 500 mg

1-Mercapto-(triethylene glycol) methyl ether functionalized gold nanoparticles solution

► **2 % (w/v) in 200 proof ethanol**

solution 

density 0.793 g/mL, 25 °C

solubility

toluene soluble
 chloroform soluble
 ethyl acetate soluble
 acetone soluble
 acetonitrile slightly soluble
 alcohol soluble
 H₂O soluble
 particle size 3.5-5.5 nm (TEM)

694169-5ML 5 mL

(1-Mercaptoundec-11-yl)tetra(ethylene glycol) functionalized gold nanoparticles solution

► **2 % (w/v) in H₂O**

solution 

solubility

alcohol soluble
 H₂O soluble
 density 1.00 g/mL
 particle size 3.5-5.5 nm (TEM)

687863-5ML 5 mL

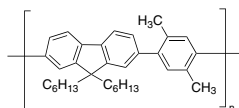
Organic Electronics

For a complete list of materials for organic electronics, please visit us at sigma-aldrich.com/oel.

Light-Emitting Polymers

Poly[(9,9-dihexylfluoren-2,7-diyl)-*alt*-(2,5-dimethyl-1,4-phenylene)]

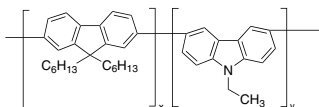
PF-DMB
[579505-48-9]



fluorescence λ_{ex} 330 nm, λ_{em} 379 nm in chloroform
mp..... >400 °C
685690-500MG 500 mg

Poly[(9,9-dihexylfluoren-2,7-diyl)-*co*-(9-ethylcarbazol-2,7-diyl)]

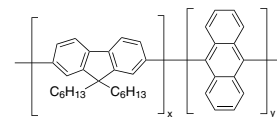
PFH-EC



fluorescence λ_{ex} 374 nm, λ_{em} 417 nm in chloroform
mp..... 111 to 122 °C
685704-500MG 500 mg

Poly[(9,9-dihexylfluoren-2,7-diyl)-*co*-(anthracen-9,10-diyl)]

[474975-22-9]

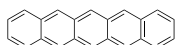


fluorescence λ_{ex} 375 nm, λ_{em} 441 nm in chloroform
mp..... 407 to 456 °C
685712-500MG 500 mg

Molecular Semiconductors

Pentacene, 99.9+% (metals basis)

$\text{C}_{22}\text{H}_{14}$
FW 278.35
[135-48-8]
EC No. 2051937
BRN 1912418



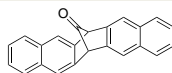
► sublimed

mp..... >300 °C
mp..... 372 to 374 °C (subl.)
transition temp (DSC trace available upon request)

684848-1G 1 g

6,13-Dihydro-6,13-methanopentacene-15-one

DMP; soluble pentacene precursor
 $\text{C}_{24}\text{H}_{14}\text{O}$
FW 318.37



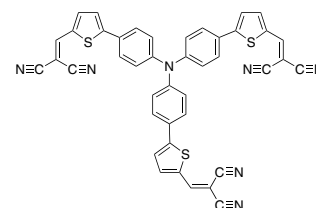
Pentacene precursor quantitatively converted to pentacene by heating at 150 °C, generating CO gas as the only by-product of the thermal conversion. Sparingly (~0.7mg/ml) soluble in apolar solvents (chloroform, toluene, THF).¹

Lit cited: 1. Chen, K.; Hsieh, H.; Wu, C.; Hwang, J.; Chow T., *Chem. Commun.* 1065 (2007)

688045-100MG 100 mg
688045-500MG 500 mg

Tris[4-(5-dicyanomethylidenemethyl-2-thienyl)phenyl]amine, 97%

TDCV-TPA
 $\text{C}_{42}\text{H}_{21}\text{N}_7\text{S}_3$
FW 719.86



Isotropic organic semiconductor for OPVs and OLED's. TDCV-TPA^{1,2} is soluble in a large variety of organic solvents and can be used for the fabrication of heterojunction solar cells with high open-circuit voltage (1.15V), efficiency close to 2% and longer ambient condition lifetimes than cells based on poly(alkylthiophenes). The compound absorbs at 509nm (in CH_2Cl_2 solution) and 538nm as thin film. It can be used as high spectral purity luminophore in LED's, emitting red light at 658nm.

fluorescence λ_{ex} 510 nm, λ_{em} 592 nm in chloroform
mp..... 400 °C

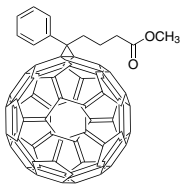
Lit cited: 1. Roquet, S.; Cravino A.; Leriche, P.; Alévêque, O.; Frère, P.; Roncali, J., *J. Am. Chem. Soc.* **128**, 3459 (2006)

2. Cravino, A.; Leriche, P.; Alévêque, O.; Roncali, J., *Adv. Mater.* **18**, 3033 (2006)

687251-100MG 100 mg

[6,6]-Phenyl C₆₁ butyric acid methyl ester

[60]PCBM
 C₇₂H₁₄O₂
 FW 910.88
 [160848-21-5]



functionalized fullerene

▶ **>99%**

684430-1G 1 g

▶ **>99.5%**

684449-100MG 100 mg

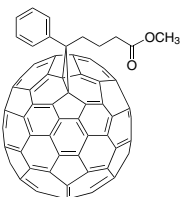
684449-500MG 500 mg

▶ **>99.9%**

684457-100MG 100 mg

[6,6]-Phenyl C₇₁ butyric acid methyl ester, mixture of isomers, 99%

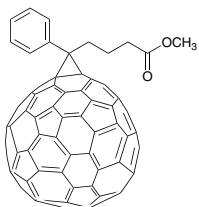
[70]PCBM
 C₈₂H₁₄O₂
 FW 1030.99
 [609771-63-3]



684465-100MG 100 mg

[6,6]-Phenyl C₈₅ butyric acid methyl ester, mixture of isomers, 99+%

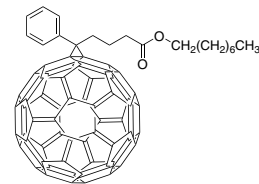
[84]PCBM
 C₉₆H₁₄O₂
 FW 1199.14
 [905843-95-0]



684473-100MG 100 mg

[6,6]-Phenyl-C₆₁ butyric acid octyl ester, ≥99%

[60]PCBM-C8
 C₇₉H₂₈O₂
 FW 1009.07
 [571177-68-9]

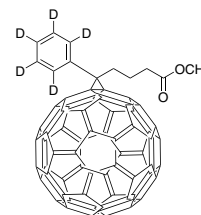


functionalized fullerene

684481-100MG 100 mg

[6,6]-Pentadeuterophenyl C₆₁ butyric acid methyl ester, 99.5%

d5-PCBM
 C₇₂D₅H₉O₂
 FW 915.91
 [749898-80-4]

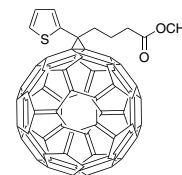
▶ **99.5 atom % D**

functionalized fullerene

684503-100MG 100 mg

[6,6]-Thienyl C₆₁ butyric acid methyl ester, 99+%

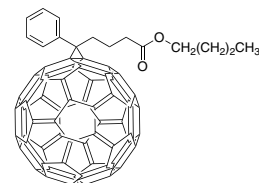
[60]ThPCBM
 C₇₀H₁₂O₂S
 FW 916.91



688215-100MG 100 mg

[6,6]-Phenyl-C₆₁ butyric acid butyl ester, >97%

PCBB; [60]PCB-C4
 C₇₅H₂₀O₂
 FW 952.96
 [571177-66-7]

▶ **>97%**

functionalized fullerene

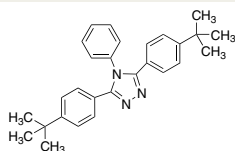
685321-100MG 100 mg

685321-1G 1 g

OLED Materials

3,5-Bis(4-tert-butylphenyl)-4-phenyl-4H-1,2,4-triazole

$C_{28}H_{31}N_3$
FW 409.57
[203799-76-2]



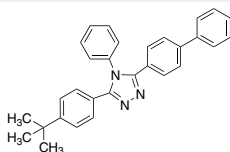
OLED electron transporter material.
97%

mp..... 224 to 229 °C

685682-1G 1 g

3-(Biphenyl-4-yl)-5-(4-tert-butylphenyl)-4-phenyl-4H-1,2,4-triazole, 97%

TAZ
 $C_{30}H_{27}N_3$
FW 429.56
[150405-69-9]



OLED¹ and QD-LED² electron transporter and hole blocker material.

fluorescence λ_{ex} 280 nm, λ_{em} 372 nm in chloroform
mp..... 231 to 235 °C

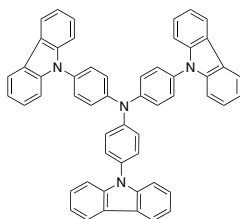
Lit. cited: 1. Kido, J.; Hongawa, K. et al., *Appl. Phys. Lett.* **63**, 2627 (1993)

2. Coe, S.; Woo, W. K. et al., *Nature* **420**, 800 (2002)

685720-1G 1 g

Tris(4-carbazoyl-9-ylphenyl)amine, 97%

TCTA
 $C_{54}H_{36}N_4$
FW 740.89
[139092-78-7]



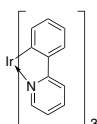
OLED hole transporter material.

mp..... 179 to 183 °C

688053-500MG 500 mg

Tris[2-phenylpyridinato-C²,N]iridium(III)

$Ir(ppy)_3$
 $C_{33}H_{24}IrN_3$
FW 654.78
[94928-86-6]



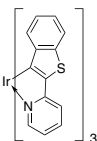
OLED triplet emitter (green).

fluorescence λ_{ex} 278 nm, λ_{em} 512 nm in chloroform

688096-250MG 250 mg

Tris[2-(benzo[b]thiophen-2-yl)pyridinato-C³,N]iridium(III)

$Ir(btpy)_3$
 $C_{39}H_{24}IrN_3S_3$
FW 823.04
[405289-74-9]



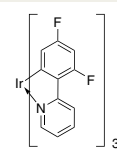
OLED triplet emitter (red).

fluorescence λ_{ex} 292 nm, λ_{em} 595 nm in chloroform
mp..... >300 °C

680877-250MG 250 mg

Tris[2-(4,6-difluorophenyl)pyridinato-C²,M]iridium(III)

$Ir(4,6Fppy)_3$
 $C_{33}H_{18}F_6IrN_3$
FW 762.72

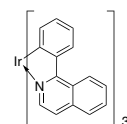


OLED triplet emitter (blue).

682594-250MG 250 mg

Tris[1-phenylisoquinoline-C²,M]iridium(III), 99%

$Ir(piq)_3$
 $C_{45}H_{30}IrN_3$
FW 804.96
[435293-93-9]



► sublimed

OLED triplet emitter (red).

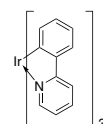
mp 454 °C

fluorescence λ_{ex} 324 nm, λ_{em} 615 nm

688118-250MG 250 mg

Tris[2-phenylpyridinato-C²,N]iridium(III)

$Ir(ppy)_3$
 $C_{33}H_{24}IrN_3$
FW 654.78
[94928-86-6]



► sublimed

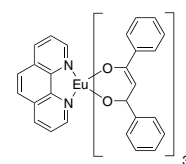
OLED triplet emitter (green).

fluorescence λ_{ex} 278 nm, λ_{em} 512 nm in chloroform

694924

Tris(dibenzoylmethane) mono(1,10-phenanthroline)europium(III)

$C_{57}H_{41}EuN_2O_6$
FW 1001.91
[17904-83-5]



► sublimed

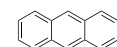
mp..... 185 to 191 °C

λ_{max} H₂O 614 nm

538965-250MG 250 mg

Anthracene, 99+%

$C_{14}H_{10}$
FW 178.23
[120-12-7]
CI 10790
EC No. 2043711
BRN 1905429



► sublimed

bp..... 340 °C

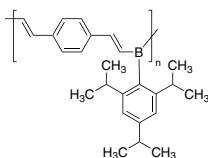
mp..... 210 to 215 °C

694959

Polymer Semiconductors

Poly[(1,4-divinylphenylene)(2,4,6-triisopropylphenylborane)]

Boramer™-T01



n-type polymer semiconductor; HOMO = -6.65 eV, LUMO = -3.85 eV.¹

fluorescence λ_{ex} 330 nm, λ_{em} 440 nm in chloroform
mp..... 103 to 112 °C

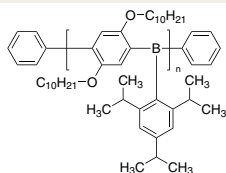
Lit. cited: 1. Luebben, S.; Sapp, S., *Material Matters* **3**, 11 (2007)

Manufactured by TDA research, Inc.

688010-250MG 250 mg

Poly[(2,5-didecyloxy-1,4-phenylene) (2,4,6-triisopropylphenylborane)], diphenyl terminated

Boramer™-T03



n-type polymer semiconductor; HOMO = -6.2 eV, LUMO = -3.0 eV.¹

fluorescence λ_{ex} 300 nm, λ_{em} 486 nm in chloroform

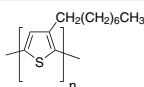
Lit. cited: 1. Luebben, S.; Sapp, S., *Material Matters* **3**, 11 (2007)

Manufactured by TDA research, Inc.

688002-250MG 250 mg

Poly(3-octylthiophene-2,5-diyl), 99.995% (metals basis)

P3OT
[104934-51-2]



► **regioregular, electronic grade, average mol wt ~25,000**

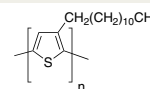
p-type polymer semiconductor.

mp..... 198 to 211 °C

682799-250MG 250 mg

Poly(3-dodecylthiophene-2,5-diyl), 99.995% (metals basis)

P3DDT
[137191-59-4]



► **electronic grade, average M_w ~27,000**

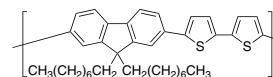
regioregular

T_m (DSC) 165.6 °C (peak)

682780-250MG 250 mg

Poly[(9,9-dioctylfluorenyl-2,7-diyl)-co-bithiophene]

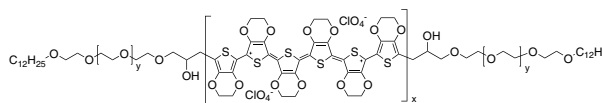
F8T2
[210347-56-1]



p-type polymer semiconductor.

685070-250MG 250 mg

Poly(3,4-ethylenedioxythiophene), bis-poly(ethyleneglycol), lauryl terminated



Aedotron™ C3-NM

C_{99}
FW 1189.06

Conducting polymer dispersion suitable for making conducting films, anti-static layers, transparent electrodes for electroluminescent lamps.

liquid (dispersion)

composition

acetonitrile 4-8 wt. %
Aedotron™- C3 polymer 0.2-0.7 wt. %
nitromethane 90-95 wt. %
proprietary processing additive 0.1-0.7 wt. %
propylene glycol 0.0-0.3 wt. %

concentration 0.4-0.9 wt. % (content of dispersion)

conductivity 10-60 S/cm

surface resistivity..... 600-3000 Ω /sq

λ 70-85%

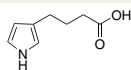
particle size..... 200-600 nm

687316-25G 25 g

Synthetic Tools

4-(3-Pyrrolyl)butyric acid, 95%

$C_8H_{11}NO_2$
FW 153.18
[30000-61-4]



mp..... 91 to 95 °C

682578-100MG 100 mg

682578-500MG 500 mg

1H-Pyrrole-1-propanoic acid, 97%

N-(2-Carboxyethyl)pyrrole; N-Pyrrolylpropanoic acid;
3-Pyrrolyl-1-yl-propionic acid
 $C_7H_9NO_2$
FW 139.15
[89059-06-3]

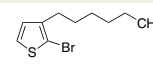


mp..... 59 to 64 °C

687545-1G 1 g

2-Bromo-3-hexylthiophene, 97%

$C_{10}H_{15}BrS$
FW 247.20
[69249-61-2]



density..... 1.240 g/mL, 25 °C

n_D^{20} 1.529

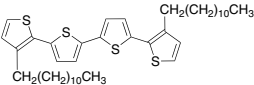
691925-1G 1 g

691925-5G 5 g

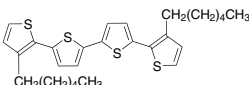
2-Bromo-3-dodecylthiophene, 95%

C ₁₆ H ₂₇ BrS	
FW 331.35	
[139100-06-4]	
density.....	1.105 g/mL, 25 °C
n _D ²⁰	1.509
688312-1G	1 g


3,3''-Didodecyl-2,2':5',2'':5'',2'''-quaterthiophene, 97%

5,5'-Bis(3-dodecyl-2-thienyl)-2,2'-bithiophene	
C ₄₀ H ₅₈ S ₄	
FW 667.15	
[162151-09-9]	
mp.....	55 to 59 °C
691631-500MG	500 mg

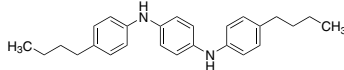
3,3''-Dihexyl-2,2':5',2'':5'',2'''-quaterthiophene

5,5'-Bis(3-hexyl-2-thienyl)-2,2'-bithiophene; DH-4T; α,ω-Dihexylquaterthiophene	
C ₂₈ H ₃₄ S ₄	
FW 498.83	
694460-1G	1 g

4,7-Dibromobenzo[c][1,2,5]thiadiazole

C ₆ H ₂ Br ₂ N ₂ S	
FW 293.97	
[15155-41-6]	
693847-1G	1 g
693847-5G	5 g

N',N''-Bis(4-butylphenyl)benzene-1,4-diamine, 97%

N,N'-Bis(4-butylphenyl)benzene-1,4-diamine	
C ₂₆ H ₃₂ N ₂	
FW 372.55	
[372200-88-9]	
mp.....	125 to 129 °C
688061-1G	1 g

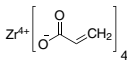
4'-(4-Chlorophenyl)-2, 2':6', 2''-terpyridine, 97%

C ₂₁ H ₁₄ ClN ₃	
FW 343.81	
[89972-75-8]	
mp.....	168 to 172 °C
687073-1G	1 g
687073-5G	5 g

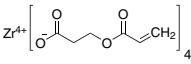
Photonics

New multifunctional zirconium and hafnium acrylate monomers will help you make high refractive index films for light management applications. For a complete list of photonic and optoelectronic materials, please visit us at sigma-aldrich.com/photronics.

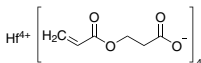
High Refractive-Index Monomers**Zirconium acrylate**

C ₁₂ H ₁₂ O ₈ Zr	
FW 375.44	
[60653-57-8]	
686239-25G	25 g

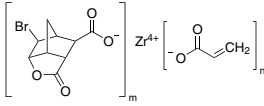
Zirconium carboxyethyl acrylate

C ₂₄ H ₂₈ O ₁₆ Zr	
FW 663.69	
[123633-53-4]	
► 60% (n-propanol)	
contains 500 ppm methyl hydroquinone as inhibitor	
bp.....	100-121 °C
density.....	1.101 g/mL, 25 °C
686247-100G	100 g

Hafnium carboxyethyl acrylate

C ₂₄ H ₂₈ HfO ₁₆	
FW 750.96	
► 60% in 1-butanol	
contains 500 ppm methyl hydroquinone as inhibitor	
density.....	1.154 g/mL, 25 °C
686220-25G	25 g

Zirconium bromonorborenelactone carboxylate triacrylate

PRM30	
average mol wt ~600	
contains 500 ppm methyl hydroquinone as inhibitor	
686204-25G	25 g

Self-Assembly Materials

For a complete list of materials for making self-assembled monolayers, please visit us at sigma-aldrich.com/selfassembly.

For Oxidic Surfaces

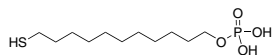
11-Mercaptoundecylphosphoric acid, 99%

11-Mercapto-1-undecyl dihydrogen phosphate

$C_{11}H_{25}O_4PS$

FW 284.35

[188678-49-1]



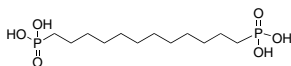
mp..... 48 to 52 °C

674311-50MG 50 mg

(12-Phosphonododecyl)phosphonic acid, 97%

$C_{12}H_{28}O_6P_2$

FW 330.29



mp..... 181 to 187 °C

685437-1G 1 g

11-Phosphonoundecanoic acid, 96%

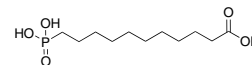
$C_{11}H_{23}O_5P$

FW 266.27

[4494-24-0]

mp..... 186 to 190 °C

678031-1G 1 g



Thiols

11-Amino-1-undecanethiol hydrochloride, 99%

$C_{11}H_{25}NS \cdot HCl$

FW 239.85

[143339-58-6]

$HSCH_2(CH_2)_9CH_2NH_2 \cdot HCl$

mp..... 120 to 170 °C

674397-50MG 50 mg

m-Carborane-9-thiol, 97%

1,7-Dicarbido-*c*-closo-dodecaborane-9-yl-thiol;

9-Mercapto-1,7-dicarbido-dodecaborane (12)

$C_{12}H_{12}B_{10}S$

FW 176.29

[64493-44-3]



mp..... 181 to 185 °C

686506-250MG 250 mg

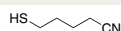
4-Cyano-1-butanethiol

5-Mercaptopentanenitrile

C_5H_9NS

FW 115.20

692581



6-(Ferrocenyl)hexanethiol

6-(Mercaptohexyl)ferrocene

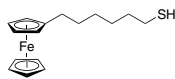
$C_{16}H_{22}FeS$

FW 302.26

[134029-92-8]

mp..... 320 °C (dec.)

682527-250MG 250 mg



11-Mercaptoundecylphosphoric acid, 99%

11-Mercapto-1-undecyl dihydrogen phosphate

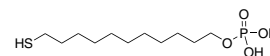
$C_{11}H_{25}O_4PS$

FW 284.35

[188678-49-1]

mp..... 48 to 52 °C

674311-50MG 50 mg



11-Mercaptoundecyl trifluoroacetate, 99%

$C_{13}H_{23}F_3O_2S$

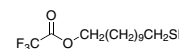
FW 300.38

[138524-05-7]

mp..... 50 to 51 °C

density..... 1.059 g/mL, 25 °C

674230-50MG 50 mg



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