Materials for Battery Applications
Redox Shuttles & Electrolyte Solvents

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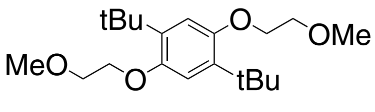
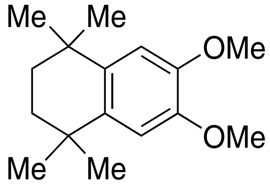
Redox Shuttles

- Provides a long-term intrinsic overcharge protection of lithium-ion batteries.
- Maintains the safe operation of lithium-ion batteries.
- Highly-soluble in conventional non-aqueous, carbonate based electrolytes.
- Increases long-term stability and oxidation potential of battery.



ANL-RS2 **08-0215**



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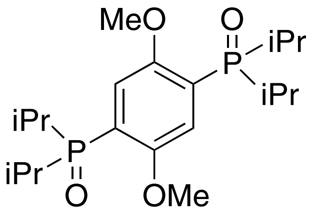

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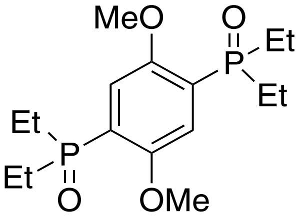

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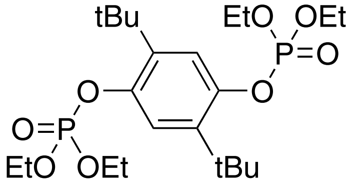
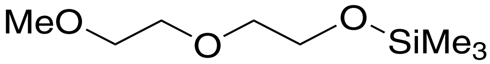


ANL-RS6 **15-1375**

Electrolyte Solvents

- Silicon based electrolytes with polyethylene glycol oligomers improve thermal and electrochemical stability of lithium-ion batteries
- Increases battery long-term stability
- Less flammable than conventional organic carbonate-based solvents and maintain the safe operation of batteries
- Improves conductivity and kinetics of lithium salts



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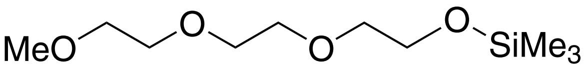

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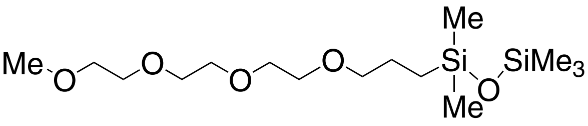
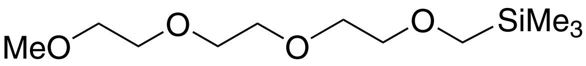


ANL-2SM3 **14-1943**



ANL-1S1M3 **14-1946**

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08-0215 **1,4-Di-t-butyl-2,5-bis(2-methoxyethoxy)benzene, 99+% Redox shuttle ANL-RS2** 1g
CAS# 1350770-63-6; $C_{20}H_{34}O_4$; F.W. 338.48; white to off-white pwdr. 5g
U.S. Patent: 8,609,287. European Patent App.: 11787270.5. Chinese Patent App.: 11/80014192.6

Technical Notes:

Electrochemical Properties:

1. ANL-RS2 (abbreviated DBBB) redox shuttle, compared to other dimethoxybenzene-based shuttles, has demonstrated improved solubility in carbonate-based electrolytes. DBBB displays a reversible redox potential at 3.9 V. [1]
2. In comparison to a variety of quinoxaline-based species, DBBB exhibits a reversible single electron transfer at 4 V vs. Li/Li+. Quinoxaline and its derivatives demonstrate two redox events between 2.4-3 V vs. Li/Li+. [2]
3. DBBB enriched electrolyte demonstrated effective protection against overcharge abuse in 18650 format $LiFePO_4$ based lithium ion batteries. [3]
4. Due to excellent solubility in carbonate-based electrolytes and improved electrolyte conductivity, DBBB is compatible with modern battery technologies. [4-5]

References:

1. *Energy Environ. Sci.*, **2012**, *5,* 8204.
2. *Adv. Energy Mater.*, **2012**, *2,* 1390
3. *J. Power Sources,* **2014**, *247,* 1011.
4. *J. Electrochem. Soc.*, **2014**, *161,* A1905.
5. *J. Electrochem. Soc.*, **2016**, *163,* A1.

08-0220 **6,7-Dimethoxy-1,1,4,4-tetramethyl-1,2,3,4-tetrahydronaphthalene, 99+% Redox shuttle ANL-RS21** 1g
CAS# 22825-00-99; $C_{16}H_{24}O_2$; F.W. 248.36; off-white solid 5g
U.S. Patent: 8,609,287. European Patent App.: 11787270.5. Chinese Patent App.: 11/80014192.6

Technical Notes:

Electrochemical Properties:

1. ANL-RS21 5 mM exhibits a redox potential of about 4.05V, in electrolytes (1.2 M LiPF6 in 3:7 wt/wt mixtures of EC/EMC. [1]
2. The redox shuttle in aprotic solvents can be used from -30° C to 70° C and are stable in the electrochemical window in which the cell electrodes and redox shuttle operates. ANL-RS21 undergoes reversible electrochemical oxidation to form stable cation-radical salts. [2]

References:

1. US 2013/0288137 A1
2. *Org. Lett.*, **2009**, *11,* 2253.

15-1365 **(2,5-Dimethoxy-1,4-phenylene)bis(di-i-propylphosphine oxide), 99+% Redox shuttle ANL-RS5** 250mg
CAS # 1426397-81-0; $C_{20}H_{36}O_4P_2$; F.W. 402.45; white pwdr. 1g
U.S. Patent: 14/171,556

Technical Notes:

Electrochemical Properties:

1. ANL-RS5 (abbreviated BPDB) exhibits a reversible redox potential of about 4.5V vs Li/Li^+ (1.2 M $LiPF_6$ in 3:7 wt/wt mixture of ethylene carbonate and ethyl methyl carbonate)[1]
2. Provides stable overcharge protection for 4V MCMB (mesocarbon microbead)/LMO ($LiMn_2O_4$) cells delivering 95 cycles of 100% overcharge at room temperature[1]

References:

1. *J. Mater. Chem., A*, **2015**, *3*, 10710.

15-1372 **(2,5-Dimethoxy-1,4-phenylene)bis(diethylphosphine oxide), 99+% Redox shuttle ANL-RS51** 500mg
CAS# 1802015-49-1; $C_{16}H_{28}O_4P_2$; F.W. 402.45; white solid 2g
U.S. Patent: 14/171,556

Technical Notes:

Electrochemical Properties:

1. ANL-RS51 exhibits a reversible redox potential of about 4.6V vs Li/Li^+ (1.2 M $LiPF_6$ in 3:7 wt/wt mixture of ethylene carbonate and ethyl methyl carbonate).

References:

1. US 20150221982 A1, 6 Aug. 2015.

15-1375 **2,5-Di-t-butyl-1,4-phenylene tetraethyl bis(phosphonate), 99+% Redox shuttle ANL-RS6** 500mg
CAS# 1350767-15-5; $C_{22}H_{40}O_8P_2$; F.W. 494.50; white solid 2g
U.S. Patents: 8,969,625

Technical Notes:

Electrochemical Properties:

1. ANL-RS6 (10 mM) exhibits a reversible redox potential of about 4.8V vs Li/Li+ (1.2 M $LiPF_6$ in 3:7 wt/wt mixtures of ethylene carbonate and ethyl methyl carbonate.[1]
2. In cell tests using $LiMn_2O_4$ and $Li_{1.2}Ni_{0.15}Co_{0.1}Mn_{0.55}O_2$ as the cathode materials, overcharge protection was provided at 4.75 V vs. Li/Li+.[1]

References:

1. *Energy Environ. Sci.*, **2011**, *4*, 2858.

14-1925 **2,2-Dimethyl-3,6,9-trioxa-2-siladecane, 99+% Electrolyte solvent ANL-1NM2** 500mg
CAS# 62199-57-9; $C_8H_{20}O_3Si$; F.W. 192.33; colorless liq. 2g
U.S. Patent: 8,475,688

Technical Notes:

Electrochemical and Physical Properties:

1. **Viscosity**: 0.9 cP at 25°C; **Conductivity**: 1.2 x 10^{-3}S cm^{-1} at 25°C (1.0 M LiTFSI); **Boiling point**: 190-191°C; **Glass transition temperature**: -129°C [1-3].
2. LiTFSI is a soluble electrolytic lithium salt. LiBOB is less soluble.
3. Silylated electrolytes show much better electrochemical stability than their carbon and germanium analogues [3].
4. Compares well with other trimethylsilylated polyethyleneoxide oligomers, with longer chain lengths (see also ANL-1NM3; product # 14-1930). Ethylene oxide units in certain electrolytic blends are advantageous improving the conductivity and kinetics of the lithium salts [3-4].

References:

1. *Electrochem. Commun.*, **2006**, *8*, 429.
2. *J. Phys. Chem. C*, **2008**, *112*, 2210.
3. *J. Mater. Chem.*, **2008**, *18*, 3713.
4. *J. Power Sources*, **2014**, *272*, 190.

14-1930 **2,2-Dimethyl-3,6,9,12-tetroxa-2-silatridecane, 99+% Electrolyte Solvent ANL-1NM3** 1g
CAS# 864079-62-9; $C_{10}H_{24}O_4Si$; F.W. 236.38; colorless liq. 5g
Use for batteries for medical devices expressly excluded. U.S. Patent: 8,076,032

Technical Notes:

Electrochemical and Physical Properties:

1. **Viscosity**: 1.4 cP at 25°C, doped with 0.8M LiBOB electrolyte 1.9 cP at 25°C; **Conductivity** of 0.8M LiBOB doped electrolyte: 1.18 x 10^{-3} S cm^{-1} at 25°C; **Thermally stable** up to 400°C. **Boiling point**: 233-234°C; **Glass transition temperature**: -116°C [1, 2].
2. Soluble electrolytic lithium salts: LiBOB, $LiPF_6$ (03-0325), $LiBF_4$ (03-0325 Strem product - not battery grade) and LiTFSI
3. ANL-1NM3 electrolytes show excellent charge/discharge cycling behavior in lithium-ion cells. Silane-based electrolytes with certain lithium salts are stable to 4.4 V [1]
4. Compared to other trimethylsilylated polyethyleneoxide oligomers (see also ANL-1NM2; product # 14-1925) with two and three ethylene oxide units, these electrolytic blends are advantageous for the conductivity and kinetics of the lithium salts [2]. In some cases, ANL-1NM3 is more preferable because of the higher boiling point (233-234°C vs 190-191°C of ANL-1NM2) and a lower viscosity.
5. ANL-1NM3 doped with lithium salts exhibit high ionic conductivity (more than 10–3 S cm–1) at room temperature. Lithium bis(oxalate)borate (LiBOB) a salt blended silicon electrolyte shows the most stable and highest electrochemical performance [3-5]. In addition, silylated electrolytes show much better electrochemical stability than carbon and germanium analogues [6].
6. Organosilicon electrolyte helps to enhance the transport properties of other electrolytes [7], shows excellent thermal and electrochemical stability [8] and also applicable for Li-air batteries [9]

References:

1. *Electrochem. Commun.*, **2006**, *8*, 429.
2. *Phys. Chem. C*, **2008**, *112*, 2210.
3. *J. Power Sources*, **2011**, *196*, 2255.
4. *J. Power Sources*, **2011**, *196*, 8301.
5. *Phys. Chem. C*, **2011**, *115*, 24013.
6. *J. Mater. Chem.*, **2008**, *18*, 3713.
7. *J. Phys. Chem. C*, **2010**, *114*, 20569.
8. *J. Power Sources*, **2013**, *241*, 311.
9. *J. Phys. Chem. C*, **2011**, *115*, 25535.

14-1943 **2,2,4,4-Tetramethyl-3,8,11,14,17-pentaoxa-2,4-disilaoctadecane, 99+% Electrolyte solvent ANL-2SM3** 1g
CAS# 864079-63-0; $C_{15}H_{36}O_5Si_2$; F.W. 352.61; colorless liq. 5g
Use for batteries for medical devices expressly excluded. U.S. Patent: 8,076,031 B1

Technical Notes:

Electrochemical and Physical Properties:

1. Disiloxane liquid electrolyte ANL-2SM3 exhibits electrochemical stability, high thermal stability, and low viscosity.- **Viscosity** 3.8 cP at 25°C; **The conductivity and viscosity** of ANL-2SM3-based electrolyte are3.65×10^{-4} S cm^{-1} and 18 cP at 25 °C [1,2]
   Charged cathode material is more thermally stable in the siloxane-based electrolyte than in the carbonate-based electrolyte [1].
   Boiling point 269-271°C; Glass transition temperature -103.0°C
2. Soluble electrolytic lithium salts: LiBOB, LiPF6, ANL-2SM3, and LiTFSIANL-2SM3 is compatible with nanostructured material based electrodes [3].
3. Disiloxane/LiBOB or Disiloxane /$LiPF_6$ electrolytes show conductivities up to 6.2×10^{-4} Scm^{-}1 at room temperature. Disiloxane electrolytes doped with 0.8MLiBOB are stable to 4.7 V. The LiBOB/disiloxane combinations were found to be good electrolytes for lithium-ion cells [4]

References:

1. *Electrochem. Commun.*, **2006**, *8,* 429.
2. *J. Mater. Chem.*, **2010**, *20,* 8224.

14-1946 **2,2-Dimethyl-4,7,10,13-tetraoxa-2-silatetradecane, 99+% Electrolyte solvent ANL-1S1M3** 1g
CAS# 864079-63-0; $C_{11}H_{26}O_4Si$; F.W. 250.41; colorless liq. 5g
Use for batteries for medical devices expressly excluded. U.S. Patent: 8,076,032

Technical Notes:

Electrochemical and Physical Properties:

1. **Viscosity**: 2.0 cP at 25°C; **Conductivity** of 0.8M LiBOB electrolyte: 1.29 x 10^{-3}S cm^{-1} at 25°C. **Boiling point**: 245°C; **Glass transition temperature**: -110°C [1, 2].
2. Soluble electrolytic lithium salts: LiBOB, LiPF6 (03-0325), and LiTFSI
3. ANL-1S1M3 is non-hydrolyzable and less flammable than its alkoxysilane counterparts [2].
4. ANL-1S1M3 electrolyte cell test demonstrated good cycling performance in lithium-ion batteries, with a charge and discharge rate of C/5, cycled between 3.0 and 4.2 V at room temperature with only 9% capacity loss over 200 cycles [2].

References:

1. *Electrochem. Commun.*, **2006**, *8,* 429.
2. *J. Mater. Chem.*, **2010**, *20,* 8224.