3M

Product Information

Fluorad™

Lithium (Bis) Trifluoromethanesulfonimide Battery Electrolyte HQ-115

Introduction

3M™ Fluorad™ lithium (Bis) Trifluoromethanesulfonimide HQ-115 is an electrolyte salt ideal for organic electrolyte-based lithium batteries.

Cyclic voltamogram studies indicate excellent electrochemical stability. The organic ion is capable of strong covalent bonding and hence exhibits excellent resistance to thermal degradation. Not only does the strong electron withdrawing power of the CF_3- groups help to delocalize the charge on the anion, but the presence of the sulfur, oxygen, and nitrogen atoms, can participate in charge dispersal to further promote dissociation. Fluorad battery electrolyte HQ-115 conductivity values similar to those of $LiClO_4$ and $LiAsF_6$ are possible without the attendant stability and safety concerns.

HQ-115 battery electrolyte has been evaluated in many emerging battery technologies with encouraging results. Papers have been published showing its utility in lithium ion cells, primary and secondary lithium cells using organic liquid electrolytes and polymer batteries.

Material Description

Not for specification purposes

Properties	HQ-115
Chemical name	Lithium (Bis) trifluoromethanesulfonimide
Formula	$(CF_3 SO_2)_2 N^- Li^+$
Cas No	90076-65-6
Appearance	White powder (Deliquescent)

Physical Properties

Not for specification purposes

All values determined at 77°F (25°C) unless otherwise specified

Properties	HQ-115
Formula weight	287
Melting point	236°C
Water content	<0.50 Wt%
pH 1% Aqueous	~7.5
Trace ions	Aluminum, boron, calcium, chloride, fluoride, iron, nickel, potassium, silicon, sodium, sulfate

3M™ Fluorad™ lithium (Bis) trifluoromethanesulfonimide HQ-115 Solubility

The solubility of Fluorad battery electrolyte HQ-115 in various solvents (at 25°C) is given below. Solubilities in many of these solvents are excellent, thus making it possible to use solvent blends to improve electrical conductivity and viscosity.

Table 1

Solvent	Solubility
1,3-Dioxolane	56
1,4-Dioxane	<25
γ-Butyrolactone	50
Diethyl Ether	63
Dimethoxyethane	63
Ethyl Acetate	63
Isopropyl Ether	50
Methyl t-Butyl Ether	63
Propylene Carbonate	46
Tetrahydrofuran	56

Stability

The thermal stability of Fluorad battery electrolyte HQ-115, as determined by thermogravimetric analysis, indicates good thermal stability to about 375°C. Independent research has confirmed that the electrochemical stability of HQ-115 battery electrolyte is excellent, demonstrating a high anodic limit. The thermogravimetric plots of typical battery electrolyte salts are shown in Figure 1.

Conductivity

In general, Fluorad battery electrolyte HQ-115 $(CF_3SO_2)_2NLi$ exhibits conductivity values which, in some solvents, can be up to five times those typically found with 3M™ Fluorad™ FC-122 CF_3SO_3Li. Figures 2, 3, and 4 illustrate the conductivity of HQ-115 battery electrolyte in typical battery solvents. HQ-115 battery electrolyte exhibits enhanced conductivity in high-ether, low dielectric solvent blends of types commonly used in lithium batteries. Published literature reports a value of 14.0 mS/cm at 25°C for a solution of DIOX:DME:PC in a 5:4:1 ratio.

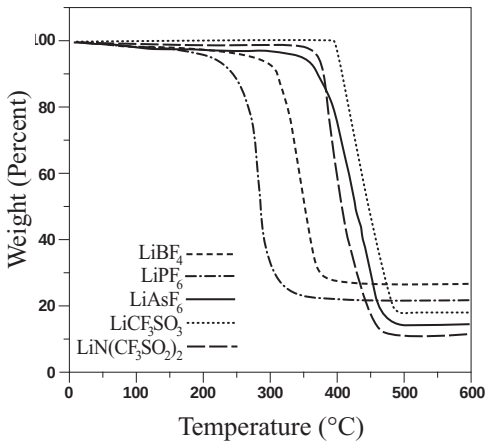

Figure 1. * Thermogravimetric analysis of Li salts under helium gas. The sample size was approximately 30 mg, the He flow rate was 50 cm^3 min^{-1} and the temperature was increased at 50°C min.

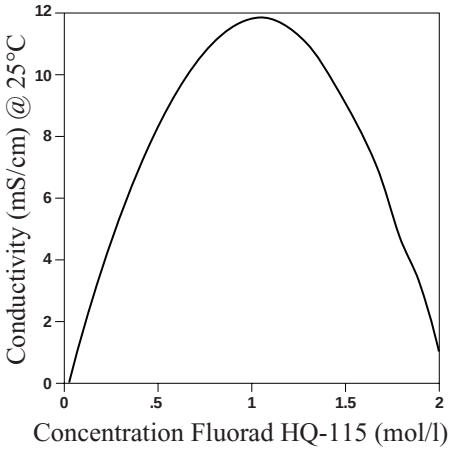

Figure 2. Conductivity of HQ-115 battery electrolyte in Dimethoxyethane at various concentrations

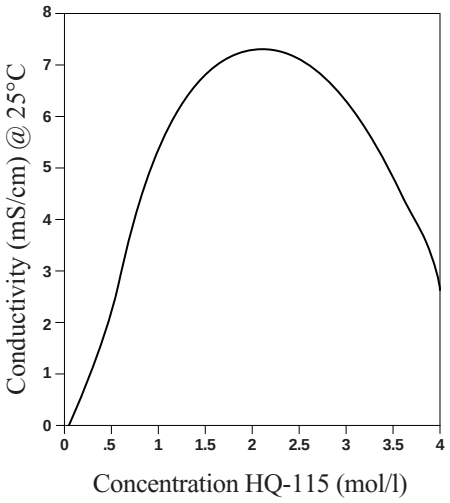

Figure 3. Conductivity of HQ-115 battery electrolyte in Dioxolane at various concentrations

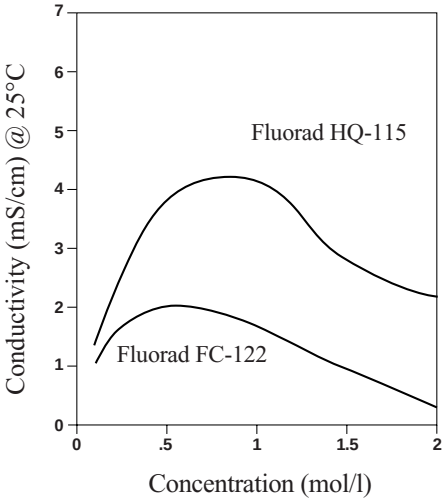

Figure 4. Conductivity of HQ-115 battery electrolyte and Fluorad FC-122 in propylene carbonate at various concentrations

Table 2 *

Conductivities of $LiN(CF_3SO_2)_2$-based non-aqueous electrolytes versus temperature

$LiN(CF_3SO_2)_2$ (M)	Electrolyte solvents			Vol. % solvent			Conductivity (mS cm^{-1}) at Celsius temperature indicated									
	1	2	3	1	2	3	-50	-40	-30	-20	-10	0	20	40	60	80
1.0	2-MeTHF	EC	PC	75	12.5	12.5		2.07		3.40	4.28	5.12	7.06	8.71	10.41	12.02
1.0	g-Butyrolactone	DME		50	50				4.30	5.72	7.35	9.19	13.13	17.33	21.60	25.43
1.0	g-Butyrolactone	Ethyl-monoglyme		50	50				2.50	3.58	4.81	6.18	9.24	12.47	15.76	18.96
1.0	DME	EC		50	50					f	5.46	7.87	12.08	16.58	21.25	25.97
1.0	DME	PC		50	50					3.92	5.44	7.19	11.23	15.51	19.88	24.30
1.0	EC	Ethyl-monoglyme		50	50					f	4.03	5.49	8.70	12.07	15.74	19.47
1.0	EC	PC		50	50		sppt	0.28	0.67	1.21	1.94	2.80	5.12	7.69	10.70	13.86
1.0	Ethyl-monoglyme	Sulfolane		50	50		0.22	0.39	0.78	1.27	1.92	2.67	4.58	6.75	8.99	11.29
0.75	Sulfolane	Triglyme		50	50				0.23	0.45	0.80	1.24	2.58	4.22	6.30	8.60

f = frozen
sppt = salt precipitation

* Journal of Power Sources 35, 59–82 (1991), "Conductivity of Electrolytes for Rechargeable Lithium Batteries," Moli Energy (1990) Ltd., 3958 Myrtle Street, Burnaby, BC, V5C 4G2 (Canada)

Drying

The salt is very hygroscopic and will deliquesce. Before its use in lithium batteries Fluorad battery electrolyte HQ-115 must be dried. Drying at 130–140°C under full vacuum is usually sufficient to reduce moisture to acceptable levels.

3M™ Fluorad™ lithium (Bis) trifluoromethanesulfonimide HQ-115 Patents

Users of lithium (bis) trifluoromethanesulfonimide are advised that some uses of this product may be covered by U.S. Patent Nos. 5,021,308 and 4,505,997 or the equivalent Japanese or European patents. Potential users should contact 3M regarding a license.

Product Safety and Handling

Please refer to the Material Safety Data Sheet and product label for safety, health, and environmental information before using product. Material Safety Data Sheets are available from your local 3M representative.

Store at or near room temperature in tightly closed containers to avoid moisture pick-up when not in use.

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