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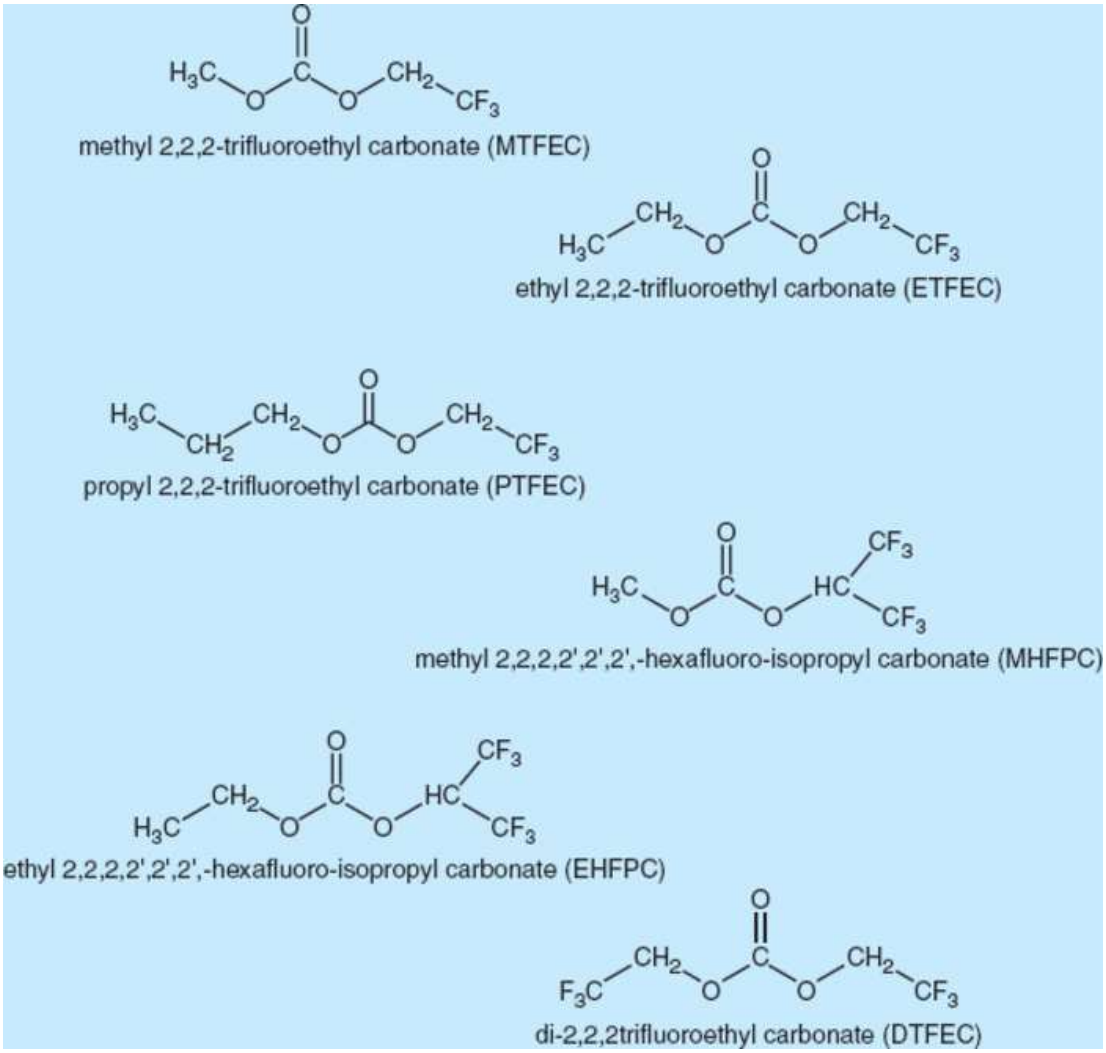
Fluorinated Alkyl Carbonates as Cosolvents in Li-Ion Cells

These solvents offer advantages with respect to performance and safety.

NASA's Jet Propulsion Laboratory

Partially fluorinated alkyl carbonate liquid compounds have been found to be excellent electrolyte cosolvents for rechargeable lithium-ion electrochemical cells. The benefits afforded by these and other ingredients of electrolyte solutions in rechargeable Li-ion cells have been investigated in continuing research directed toward extending the range of practical operating temperatures of the cells (from +40 °C down to –40 °C, and possibly even as low as –60 °C). Fluorinated solvents were perceived to be especially attractive in that they will result in inherently safer cells, due to their low flammability. This research at earlier stages was reported in a number of previous NASA Tech Briefs articles; namely, "Update on Electrolytes for Low-Temperature Lithium Cells" (NPO-20407 [/component/content/article/tb/pub/techbriefs/materials/6696]), Vol. 24, No. 1, (January 2000), page 56; "Lithium Alkoxide Electrolyte Additives for Lithium-Ion Cells" (NPO- 20607 [/component/content/article/tb/pub/techbriefs/materials/7359]), Vol. 25, No. 6 (June, 2001), page 52; "Aliphatic Ester Electrolyte Additives for Lithium-Ion Cells" (NPO-20601 [/component/content/article/tb/pub/techbriefs/materials/7360]), Vol. 25, No. 6 (June, 2001), page 53; "Ethyl Methyl Carbonate as a Cosolvent for Lithium-Ion Cells" (NPO-20605 [/component/content/article/tb/pub/techbriefs/materials/7361]), Vol. 25, No. 6 (June, 2001), page 53; and "Alkyl Pyrocarbonate Electrolyte Additives for Li-Ion Cells" (NPO-20775 [/component/content/article/tb/pub/techbriefs/materials/3168]), which precedes this article.



These Partially Fluorinated Alkyl Carbonates were tested as electrolyte cosolvents for rechargeableLi-ion cells.

The partially fluorinated carbonate cosolvents and the electrolytes formulated by use of these solvents were evaluated in comparison with baseline (nonfluorinated) alkyl carbonate cosolvents and the corresponding baseline electrolyte formulation. The baseline mixture of cosolvents consists of equal volume parts of ethylene carbonate (EC), dimethyl carbonate (DMC), and diethyl carbonate (DEC). The baseline electrolyte formulation is a 1.0 molar solution of lithium hexaflurophosphate ($LiPF_6$) in the baseline mixture of cosolvents.

The partially fluorinated carbonate solvents studied (see figure) include:

- methyl 2,2,2-trifluoroethyl carbonate (MTFEC),

- ethyl 2,2,2-trifluoroethyl carbonate (ETFEC),
- propyl 2,2,2-trifluoroethyl carbonate (PTFEC),
- methyl 2,2,2,2´,2´,2´-hexafluoro-isopropyl carbonate (MHFPC),
- ethyl 2,2,2,2´,2´,2´-hexafluoro-isopropyl carbonate (EHFPC), and
- di-2,2,2-trifluoroethyl carbonate (DTFEC).

Ternary and quaternary mixtures containing various combinations of these cosolvents were used to formulate electrolytes containing $LiPF_6$ at concentrations of 0.5, 0.75, and 1.0 molar.

The fluorinated carbonate cosolvents exhibit the requisite chemical stability of the baseline cosolvents while offering more desirable physical properties imparted by the presence of the fluorine substituents. These more desirable properties include: (1) lower melting temperatures; (2) greater chemical and electrochemical stability; (3) lower intermolecular forces and lower polarizability, which result in lower surface energies; and (4) lower flammability and thus greater safety.

Laboratory test cells constructed with these electrolytes exhibited high capacities at temperatures from –20 °C to –40 °C, capability for high rates of charge and discharge at low temperatures, and low electrode polarization. Hence, these electrolytes appear to be useful for constructing rechargeable lithium-ion cells with high specific energies, long lifetimes, and ability to function well at low temperatures.

This work was done by Marshall Smart, Ratnakumar Bugga, Subbarao Surampudi, Surya Prakash, and Jinbo Hu of Caltech for NASA's Jet Propulsion Laboratory. For further information, access the Technical Support Package (TSP) free on-line at www.nasatech.com/tsp under the Materials category. NPO-21076

This Brief includes a Technical Support Package (TSP).

Unfortunately the TSP ***Flourinated Alkyl Carbonates as Cosolvents in Li-Ion Cells*** (reference NPO-21076) appears to be missing from our system.

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