

## Bis(2,2,2-triFluoroEthyl) MethylPhosphonate as Flame-Retardant for Safer Lithium-Ion Batteries

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**Abstract:** To reduce the flammability of lithium-ion battery electrolytes, the fire suppressant effect of bis(2,2,2-trifluoroethyl) methylphosphonate (BtFEMP) was investigated experimentally. BtFEMP has a structure similar to diethyl carbonate (DEC), which is a very common component of battery electrolytes. This similar structure should allow for an integration of the fire suppressant without excessive degradation of the battery performance. The high-temperature chemistry of BtFEMP (here, between 1270 and 1700 K) was investigated in a heated shock tube (363 K) by measuring ignition delay times (IDTs) for a BtFEMP/O<sub>2</sub> in 99% Ar mixture at an equivalence ratio of 1.0 and near 1.5 atm. BtFEMP's fire suppressant potential was also assessed by measuring the effects of a small BtFEMP addition on the IDTs of well-known fuels, namely H<sub>2</sub> and CH<sub>4</sub>. To this end, H<sub>2</sub>/O<sub>2</sub> and CH<sub>4</sub>/O<sub>2</sub> in 97.9% Ar mixtures seeded with 10% of the fuel concentrations as BtFEMP were tested at three equivalence ratios ( $\phi = 0.5, 1.0, \text{ and } 2.0$ ) for temperatures ranging from 1386 to 1852 K and from 1466 to 2119 K, respectively, at near-atmospheric pressure. They are compared to H<sub>2</sub>/O<sub>2</sub> and CH<sub>4</sub>/O<sub>2</sub> IDT baselines available in the literature that were performed in similar conditions. The BtFEMP thermodynamic data were determined using *ab initio* calculations, and a detailed kinetics mechanism is under development to better highlight the role of the fluorine and phosphorus chemistry in these new global kinetics results.

**Topic Keywords:** Fire Suppressant; Bis(2,2,2-triFluoroEthyl) MethylPhosphonate; Shock Tube; Ignition Delay Times; Oxidation.