

Exploration of the Effects of Bis(2,2,2-trifluoroethyl) Methylphosphonate on the Laminar Flame Speed of Hydrogen

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Abstract: Fluorinated alkyl phosphonate compounds (FPCs) are additives that have the potential to reduce the flammability of lithium-ion battery (LiB) electrolytes. The electrolytes are frequently the reason behind LiB fires. This characteristic can be due to faulty construction of the battery or by operational abuse. Bis(2,2,2-trifluoroethyl) methylphosphonate (BtFEMP) is an FPC that is a fire suppressant candidate for usage in LiBs. Other fire suppressant candidates exist such as organophosphorous compounds (OPCs). OPCs such as trimethyl phosphate (TMP) also reduce the flammability of LiB electrolytes. However, TMP struggles to form a stable solid electrolyte interphase (SEI) on graphite anodes which increases electrolyte decomposition. In FPCs, organofluorides are helpful for forming a stable SEI. Due to this property, there is interest in the laminar flame speed (LFS) of BtFEMP for use in LiBs. However, there are no LFS studies for BtFEMP. This work will study the effects of 0.5% by volume BtFEMP on the LFS for H₂-air mixtures. It will show the LFS of BtFEMP-doped H₂-air mixtures at equivalence ratios ranging from 1.0 to 2.0 and compare the results with a baseline H₂-air mixture. All tests were conducted at an initial pressure of 1 atm and an elevated temperature of 335 K. Since there is no kinetics mechanism for FPCs, the Lawrence Livermore National Laboratory's OPC mechanism was used to approximate the numerical LFS results in Chemkin Pro. These numerical results are compared with the experimental data to show the mechanism's capacity to estimate the LFS of BtFEMP-doped H₂-air mixtures.