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$Li_{14}(PON_3)_2O$: Computational study of a possible new electrolyte for Li ion batteries[1] AHMAD AL-QAWASMEH, N. A. W. HOLZWARTH, Wake Forest Univ — Recently, $Li_{14}(PON_3)_2O$, containing Li_6PON_3 and Li_2O groups within a trigonal crystal structure (space group $P\bar{3}$ (#147)) has been synthesized by Baumann and Schnick.[2] We report the results of a first principles computational study of this material in comparison with other crystalline electrolytes having LiPON composition and iosolated tetrahedral oxonitridophosphate ions such as Li_3PO_4 and Li_7PN_4. The structure of $Li_{14}(PON_3)_2O$ is characterized by a relatively large Li ion density (0.07 Li/Å^3) which is between that of Li_3PO_4 (0.04 Li/Å^3) and Li_2O (0.09 Li/Å^3). Using a nudged elastic band approach, we find Li ion migration barriers in $Li_{14}(PON_3)_2O$ to be comparable or lower than those of Li_3PO_4 and Li_7PN_4. The most efficient migration appears to occur via a vacancy mechanism with net motion within planes perpendicular to the c-axis in the vicinity of the O sites. Models of interfaces of $Li_{14}(PON_3)_2O$ with Li metal were also studied.

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[2]Baumann and Schnick, **Eur. J. Inorg. Chem. 2015**, 617-621 (2015)

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