A Crystallographic Examination of Dilithium Phthalocyanine

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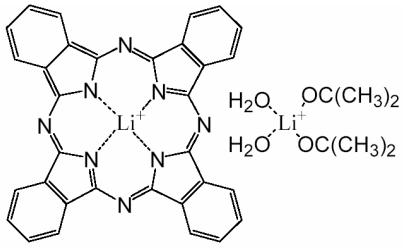
Dilithium phthalocyanine is a compound that shows promise as the dielectric for lithium-lithium ion batteries. The compound forms small, flakey crystals from the few solvents in which it can be dissolved. Experimental evidence indicates that the lithium atoms within the solid structure migrate in the presence of an electric field. The determination of the crystal and molecular structure was initiated so as to determine the pathways through which the lithium ions move.



A=12.8017(6), b=14.3637(7), c=17.3859(8), α=101.5838(9), β=94.1351(9), γ=92.3054(9), V=3118.7(3), λ=0.71073Å, T=173K, R_{int}=0.0187, R_1=0.0484, wR_2=0.1351, S=1.046, Obs=18798, Par=1116.

Keywords: battery materials, crystal structure determination, lithium batteries