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Crystal Structure of Ethylene Carbonate

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Performance and safety/stability of Li-ion batteries can be improved by either optimizing the charge storing electrodes or the charge transfer mediating liquid electrolytes. Most of the research since the commercialization of Li-ion batteries by Sony in 1991 has been focused on the electrodes and less on the electrolytes. An important class of solvents used in electrolytes are linear and cyclic carbonates, because of their good physicochemical and electrochemical properties when mixing two or more of them together with lithium salt. Thereby, ethylene carbonate (EC) is a vital part of the electrolyte with its ability to form the solid electrolyte interface, avoiding exfoliation of the graphite anode.[1] After the determination of the crystal structure of EC from single crystals[2,3] this contribution presents room temperature data obtained by Neutron Powder Diffraction at SPODI (FRM II), Total Scattering and temperature dependent Powder X-Ray Diffraction data obtained at beamline P02.1 (DESY).

[1] B. Flamme et al., Guidelines to design organic electrolytes for lithium-ion batteries: environmental impact, physicochemical and electrochemical properties, *Green Chem.* 19, 1828-1849 (2017).

[2] C.J. Brown, The Crystal Structure of Ethylene Carbonate, *Acta Cryst.* 7, 92-96, (1954).

[3] P. M. Matias et al., Single Crystal Neutron Diffraction Analysis (15K) and ab initio Molecular Orbital Calculations for Ethylene Carbonate, *Journal of Molecular Structure (Theochem)* 184, 247-260 (1989).

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