Conformational constraint in ferroelectric liquid crystals incorporating a pyrrolidine-type ring: FLC materials comprising parallel dipolar moments Ely, Fernando Cristiano, Rodrigo Longo, Ricardo L. Vergara-Toloza, Rafael Soto-Bustamante, Eduardo

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Ferroelectric liquid crystals bearing a chiral pyrrolidine-type ring were prepared using (-)-(S)-malic acid as a building block. The compounds were characterized using the thermal analysis techniques of DSC and POM, electrical measurements and temperature-dependent XRD. Samples showed moderate spontaneous polarization values (P S) with helical pitches of about 2.997 ?m and an average tilt angle of 16.2° for the SmC* planes. Conformational analysis of the chiral pyrrolidinol subunit and of all of the mesogenic targets was performed using several quantum methods including large basis sets and different treatments of electron correlation in order to correlate experimental results and theoretical predictions. For the most stable conformations, a very small dipole moment component perpendicular to the tilt plane was found which, according to the Boulder model, may be responsible for the moderate PS values obtained. © 2007 Taylor & Francis.