Optical and Pyroelectric Properties and Structure of 2[K+H(C4H5O5)-].C4H6O5

Maria Margarida R. Costa[a], Vitor Hugo Rodrigues[a], Etelvina de Matos Gomes[b], Michael S. Belsley[b], Arunhozi Gnanasundaram[b], Alberto Criado[c], *[a]CEMDRX, Departamento de Física, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, 3004-516 Coimbra, Portugal. [b]Departamento de Física, Universidade do Minho, Campus de Gualtar 4710-057, Braga, Portugal. [c]Departamento de Física de la Matéria Condensada, Universidad de Sevilla, Apartado 423566 Sevilla, Spain.* E-mail: guida@pollux.fis.uc.pt

The semi-organic crystal Bis (Potassium Hydrogen L-Malate) L-Malic Acid, 2[K+H(C4H5O5)-].C4H6O5, shows a large spontaneous polarization (in the range 30-40mC/cm2) in the vicinity of 365K, which is one order of magnitude higher than that of TGS. The title compound also shows a second harmonic generation that is about 70% that of KDP. The crystal structure has been re-determined by single crystal X-ray diffraction at 270 K and the unit cell was found to be triclinic instead of orthorhombic, as reported before[1]. Hydrogen L-malate anions form infinite head-to-tail chains via O-H…O interactions and can be used as structural building blocks in solid state crystal engineering. The neutral malic acid molecules establish links between neighbouring chains. Further structural and physical properties characterization of a similar compound, in which potassium is partially substituted by rubidium, is in progress.

[1] Van Havere W.K.L., Deukrskens P.T., Lenstra T.H., Crystall. J., *Spect. Res.*, 1985, **15**, 45.

Keywords: pyroelectricity, crystal structure analysis, optical activity