

Structure of N,N-dimethylaminopyridinium L-malate

Alberto Criado^a, M.D. Estrada^a, S. Pérez-Garrido^a, M.J. Diáñez^a, E. de Matos Gomes^b, M.S. Belsley^b, C.M.G. Miranda^b, F. Proenca^c, ^a*de la Materia Condensada, Instituto de Ciencia de Materiales, Universidad de Sevilla-CSIC, Sevilla, Spain.* ^b*Departamento de Física, Universidade do Minho, Braga, Portugal.* ^c*Departamento de Química, Universidade do Minho, Braga, Portugal.* E-mail: criado@us.es

The crystal structure of a new *L*-malic acid salt, N,N- dimethylaminopyridinium *L*-malate has been determined at room temperature using single crystal X-ray diffraction techniques. The space group is orthorhombic $P2_12_12_1$ with lattice parameters $a= 7.461(1)$, $b= 7.945(1)$ and $c= 20.774(4)\text{\AA}$. Similarly to other *L*-malic salts, the malate anions form hydrogen-bonded head-to-tail (carboxylic and carboxylate groups) infinite chains parallel to the $[100]$ crystal direction. On the other hand, the dimethylaminopyridinium cations are arranged with their mean plane approximately perpendicular to the $[100]$ crystal direction. The N-H group of every cation forms two hydrogen bonds with oxygen atoms of different anion chains connecting *L*-malate chains along the $[010]$ crystal direction. The whole crystal packing can be viewed as parallel two-dimensional hydrogen-bonded molecular arrangements perpendicular to the $[001]$ direction. As in other *L*-malic salts, preliminary measurements show optical second-harmonic generation.

Keywords: nonlinear optical materials, molecular crystals, crystal engineering