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Study of nonlinear optical crystals: L-nitroarginine perchlorate and L-nitroarginine tetrafluoroborate

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The subject of the present study is nonlinear optical (NLO) crystals: L-nitroarginine perchlorate (L-NNA·HClO4) (I) and L-nitroarginine tetrafluoroborate (L-NNA·HBF4) (II). The crystal and molecular structure of (I) and (II) crystals were determined by the single crystal X-ray diffraction method at 120K. These crystallize in the monoclinic system with space group P21 and Z=2. Unit cell parameters: a=5.1962(10) Å, b=17.903(4) Å, c=7.0030(14) Å, α=γ=90°, β=92.96(3)°, V=650.6(2) Å3 for (I) and a=5.2329(10) Å, b=18.024(4) Å, c=6.8238(14) Å, α=γ=90°, β=92.94(3)°, V=642.8(2) Å3 for (II). The (I) and (II) crystals have an isostructural structure as in the analog salts of arginine: {L-Arg·HClO4 [1] and L-Arg·HBF4 [2] with space group P212121} and {L-Arg·2HClO4 and L-Arg·2HBF4 with space group P1 [3, 4]}. The vibrational spectra (Fourier transform infrared and Raman), transparency range, thermal properties, and NLO activity of (I) and (II) crystals were studied. The NLO activities of the (I) and (II) crystals are two times higher than that of the analog salts of arginine. The (I) and (II) crystals were grown as bulk single crystals.

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