MS35-P05 | GRAPH-SET ANALYSIS AND NON-LINEAR OPTICAL PROPERTIES OF SALTS OF L-ARGININE HOMOLOGUE

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Salts of L-arginine have wide applications in medicine, such as: treatment of hepatic and renal disorders or reducing blood cholesterol [1]. They have also potential application as an energy converter in optics, because the L-arginine salts crystallize without a centre of symmetry. We present five new compounds based on the arginine homologue, (S)-2-amino-3-guanidinopropanoic acid (AmGP), as potential new functional materials: $(H_2AmGP)Cl_2$ (**1**), (HAmGP)Cl (**2**), $(H_2AmGP)(NO_3)_2$ (**3**), $(H_2AmGP)_2(H_2O)(NO_3)_4$ (**4**), $(H_2AmGP)Br_2$ (**5**). Generally, most important parts of AmGP molecule in SHG context are carboxyl and guanidinium functional groups as they possess delocalized p electrons. In the AmGP molecule, these groups are less separated to each other, and therefore higher values of hyperpolarizability β is expected for AmGP molecule in comparison to L-arginine. SHG measurements shows that the monochloride salt has 2.4 times better SHG response than KDP. What is more, (*S*)-2-amino-3-guanidiniumpropanoic acid monochloride has 8 times better SHG response than L-argininium monochloride [2]. Analysis of molecular structure reveals that conformation of the organic cation varies in presented compounds and the greatest difference occurs in (HAmGP)Cl (**2**). This fact can be associated with enhancement of SHG signal for this compound.

[1] M Walser - US Patent 4,320,146, 1982
[2] D. Kalaiselvi, Rangasamy Mohan Kumar, R. Jayavel, Crystal Research and Technology, 2008, 43:851