

Assembly of two new hybrid chloride materials with potential NLO properties: Structure elucidation, empirical and computational studies

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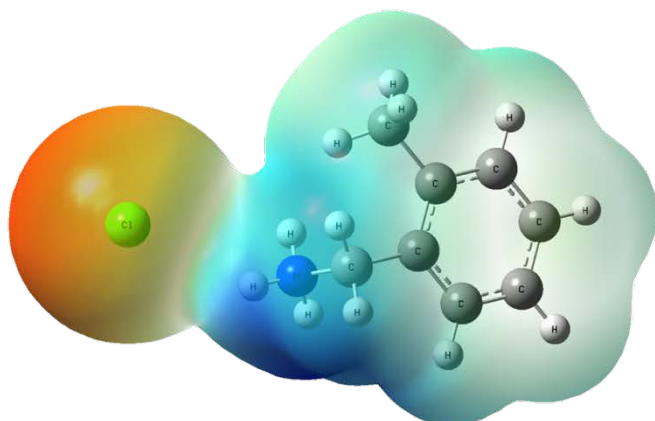
Figure captions

Fig. S1. Molecular electrostatic potential surface (MEPs) of compound 1 **(a)** and compound 2 **(b)**.

Fig. S2. DTA and TG curves of compound 1 **(a)** and compound 2 **(b)**.

(a)

$-0.151e^{-2}$  $0.151e^{-2}$



(b)

$-0.162e^{-2}$  $0.162e^{-2}$

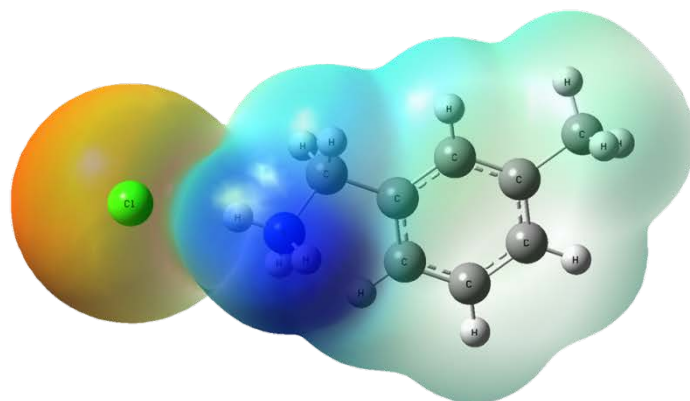
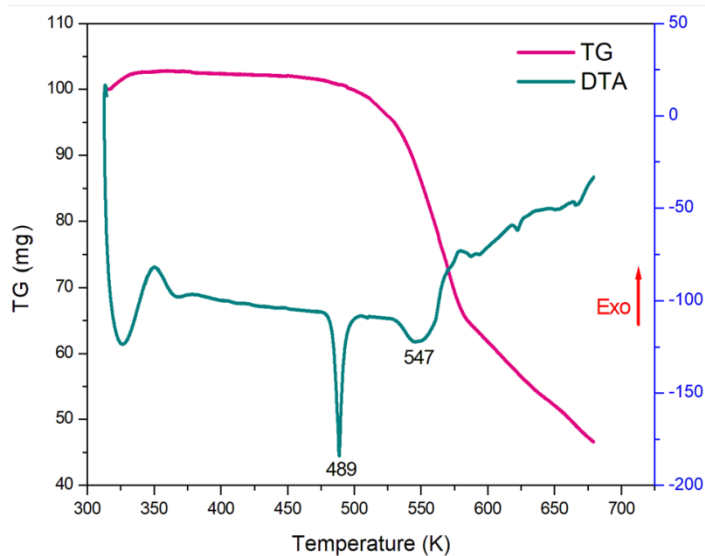


Fig. S1. Molecular electrostatic potential surface (MEPs) of compound 1 (a) and compound 2 (b).

(a)



(b)

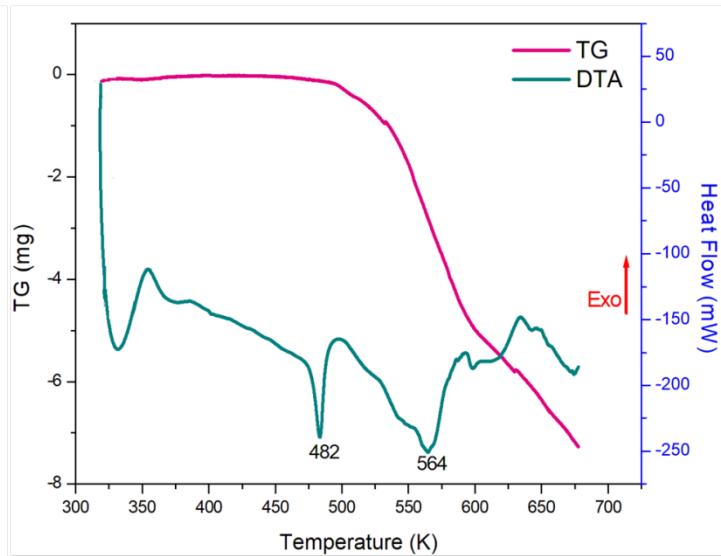


Fig. S2. DTA and TG curves of compound 1 (a) and compound 2 (b).

Table captions

Table S1. The electric dipole moment (μ), polarizability (α), and first order hyperpolarizability (β) values of compound 1.

Table S2. The electric dipole moment (μ), polarizability (α), and first order hyperpolarizability (β) values of compound 2.

Table S1. The electric dipole moment (μ), polarizability (α), and first order hyperpolarizability (β) values of compound 1.

Parameters	Value	Parameters	Value
α_{xx}	-90.7160	β_{xxx}	98.7015
α_{xy}	10.7000	β_{xxy}	-25.2212
α_{xz}	-9.4917	β_{xyy}	-7.6179
α_{yy}	-56.9405	β_{yyy}	-21.7770
α_{yz}	0.8233	β_{xxz}	6.8163
α_{zz}	-70.9019	β_{xyz}	-2.2313
α_{total} (esu)	72.8528 a.u.	β_{yyz}	0.6526
μ_x	5.6376	β_{xzz}	-2.6044
μ_y	-4.6541	β_{yzz}	-5.9841
μ_z	2.0740	β_{zzz}	6.9994
μ_{total}	7.5990	β_{total} (esu)	104.139448 a.u.

Table S2. The electric dipole moment (μ), polarizability (α), and first order hyperpolarizability (β) values of compound 2.

Parameters	Value	Parameters	Value
α_{xx}	-97.4767	β_{xxx}	-185.6928
α_{xy}	3.7622	β_{xxy}	9.7948
α_{xz}	0.6661	β_{xyy}	-3.1848
α_{yy}	-63.7134	β_{yyy}	4.4556
α_{yz}	0.4344	β_{xxz}	6.8282
α_{zz}	-70.0909	β_{xyz}	-0.9456
α_{total} (esu)	77.09366 a.u.	β_{yyz}	2.0661
μ_x	-6.5111	β_{xzz}	13.2668
μ_y	0.3438	β_{yzz}	-3.0425
μ_z	1.1246	β_{zzz}	6.4108
μ_{total}	6.6165	β_{total} (esu)	176.63243 a.u.