Cyanurates with new types of π-conjugated anions for optical materials

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The compounds containing π-conjugated units, that exhibit very large anisotropic polarizability and second harmonic generation susceptibility, can be employed as birefringent and nonlinear optical (NLO) materials. For example, the β-BBO crystal has excellent NLO properties while α-BBO is a famous ultraviolet birefringent crystal. The outstanding linear and NLO properties of them are stemmed from the planar π-conjugated $(B_3O_6)^{3-}$ groups. Recently, cyanurates containing planar $(C_3N_3O_3)^{3-}$ six-membered-ring (6-MR) units that are isoelectric with $(B_3O_6)^{3-}$ groups, can be considered as new types birefringent and NLO materials. In this talk, we have grown dozens of new cyanurates for linear and NLO applications. The noncentrosymmetric compounds show considerable NLO effects. The centrosymmetric compounds possess strong optical anisotropy, larger than that of the benchmark birefringent crystal calcite. All results show that cyanurates containing π-conjugated 6-MR groups are promising optical crystalline materials.

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