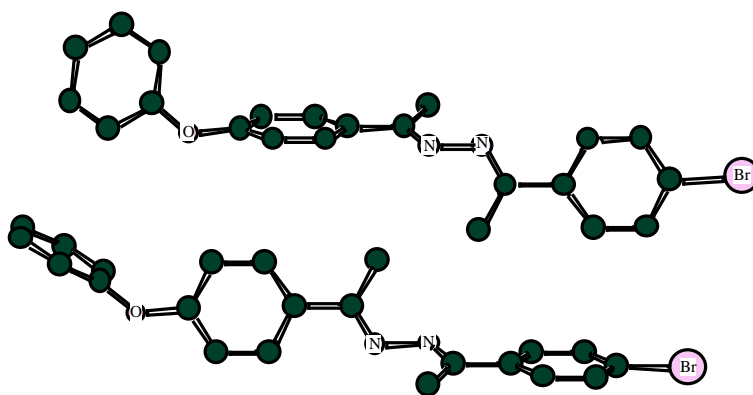


# EXPERIMENTAL REALIZATION OF TRIPLE T-CONTACTS: AN IMPROVED DESIGN FOR PREPARING DIPOLE PARALLEL- ALIGNED CRYSTALS

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Our group has been interested in the crystal packing of symmetric and asymmetric acetophenone azines.<sup>1</sup> These azines have the general formula X-Ph-C(Me)=N-N=C(Me)-Ph-Y, and they are called symmetric if X = Y and asymmetric if X ≠ Y. Our interest in these molecules stems from their ability to form dipole parallel-aligned crystals. The design of highly polar materials is important for numerous optical and electrical properties. For instance, a macroscopic dipole moment is essential for nonlinear optical (NLO) activity and this has important implications for information technologies.<sup>2</sup>



The original design concept employed dipole minimization and arene-arene quadrupole interactions to achieve dipole parallel-alignment. The central packing motif in these systems consisted of double T-contacts. We have improved this design by using phenoxy donor substituents and thus allowing for the formation of triple T-contacts (see figure). The formation of triple T-contacts greatly enhances the preference for dipole parallel-alignment because only in the dipole parallel-aligned orientation can the triple T-contact be realized. Dipole antiparallel-alignment would give the energetically less favorable double T-contact.

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2 Kanis, D. R.; Ratner, M. A.; Marks, T. J. *Chem. Rev.* **1994**, *94*, 195.