Introduction

What is a polar crystal?

A polar crystal is an ordered array of molecules in which all of the dipoles are aligned. This imparts an electronic anisotropy throughout the crystal lattice.

Polar crystals have numerous applications, including use as:

- Piezoelectrics
- Ferroelectrics
- Non-linear optical materials

A Serendipitous Discovery: mPD-Cl(OMe) Gives Aligned Dipoles in its Crystal

The Stacked Layers

The Hydrogen-Bonded Layer

Polar mPD Analogs

Non-Polar mPD Analogs

Synthetic Manipulation to Lock the Closed Conformation

mPD-H(OMe)mac: Polar Order by Rational Design

Conclusion

- We have synthesized a series of m-phenylenediamine derivatives which exhibit a preference for polar ordering.

- For the mPD synthon, a closed conformation is required for the formation of a polar crystal lattice.

- We have the ability to synthetically lock an mPD analog into this prerequisite conformation, resulting in a rationally designed polar crystal.