MS14-1-6 Screening the Cambridge Structural Database for ferroelectric molecular crystals
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Abstract
The Cambridge Structural Database (CSD) holds more than 400 000 molecular crystal entries. Many of these crystals could hold great potential as functional materials, including for applications such as photovoltaics, energy harvesting, and computer memory. Recently, organic ferroelectrics have attracted much attention due to the need for environmentally friendly ferro- and piezoelectric materials. However, identifying which of these structures merits further investigation can be challenging due to the complex structure-property relationships of ferroelectrics, requiring both an intrinsic polarization and a well-defined polarization switching path. Here, we utilize existing and newly developed tools to extract a pool of material candidates for further assessment with density functional theory. Implemented filters include the existence of pseudo-centre of symmetry and well-defined switching paths for proton-transfer ferroelectrics. For order-disorder ferroelectrics, we introduce geometric and bonding criteria to identify candidates. Moreover, we assess the potential of selected candidates using van der Waals' density functional theory. The results indicate that several candidates hold a sizeable spontaneous polarization and modest switching barriers.

Polarization switching of a proton-transfer FE