A Database for Crystalline Organic Conductors and Superconductors

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We present a prototype database for quasi two-dimensional crystalline organic conductors and superconductors based on molecules related to bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF). The database includes crystal structures, calculated electronic structures, and experimentally measured properties such as the superconducting transition temperature and critical magnetic fields. We obtained crystal structures from the Cambridge Structural Database and created a crystal structure analysis algorithm to identify cation molecules and execute tight binding electronic structure calculations. We used manual data entry to encode experimentally measured properties reported in publications. The database can be accessed through a website at osd.clarku.edu. Crystalline organic conductors and superconductors exhibit a wide variety of electronic ground states, particularly those with correlations. We hope that this database will ultimately lead to a better understanding of the fundamental mechanisms of such states.

References

1. Owen Ganter, Kevin Feeny, Morgan Brooke-deBocke, Stephen Winter, and Charles Agosta. *Crystals* **12**(7), 919 (2022).