Poster

Comparative analysis of the magnetic properties of organic compounds without metal atoms and their molecular and crystal structures

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The Cambridge Structural Database (CSD) [1] is the most comprehensive collection of information on the crystal structures of organic compounds. In addition to crystallographic data, CSD records may contain supplementary information about the shape of the crystals, the conditions for their preparation or their properties. The melting points of the crystals and their colors are indicated explicitly, but for other properties there are some short remarks only, and for acquaintance with the numerical values it is necessary to refer to the original publications.

The magnetic properties of crystals of organic compounds are usually due to the presence of metal atoms, but a certain group of compounds (radicals) reveals magnetic (mostly weak paramagnetic) properties even in the absence of metals. In the last twenty years, about two hundred crystals of such compounds have been obtained (Fig. 1), for which the presence of magnetic properties is noted in the CSD.

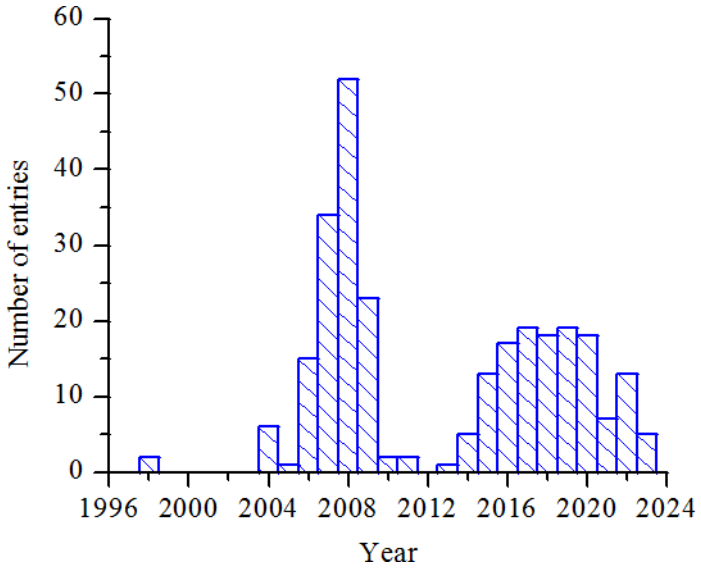

Figure 1. Distribution of the number of entries in the CSD (ver. 5.45) having a remark about magnetic properties by year for compounds without metal atoms.

In this work, the magnetic properties of compounds without metal atoms are compared with their molecular and crystal structures based on the CSD data and information found in the original publications. The collected material represents a small database, which can be supplemented as new substances are synthesized and studied.

[1] Groom, C. R., Bruno, I. J., Lightfoot, M. P., Ward, S. C. (2016). *Acta Crystallogr., Sect. B* **72**, 171.