Statistical analysis of coordination environments of metals in organic and organometallic crystals

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The use of crystallographic databases makes it possible to obtain generalized information about the crystal structure of various classes of chemical compounds. When describing the structure of substances containing metal atoms, the analysis of the coordination environment of these atoms is essential. For crystals of inorganic compounds, the coordination environment of a wide range of metal elements in oxides was considered [1], but for substances containing organic molecules or fragments of molecules, such a general study could not be found.

In this work, coordination environments of metal elements based on the CSD data (version 5.43 with 3 updates) were analyzed. Several subsets were formed, including taking into account the number of different structural residues in the unit cell (NRes) and the types of bonds (any, only with nonmetal atoms, only with metal atoms, etc.) that form the coordination environment of metals. On Fig. 1 denotes the metal elements for which there are data in the CSD related to some of the subsets considered.

Figure 1. Metal elements occurring in the subsets with NRes > 1 and any type of bonds (left) or having at least one metal-to-metal bond (right).

It turned out, in particular, that the maximum coordination number is 20. Examples of molecules with such coordination are shown in Fig. 2.

Figure 2. Examples of molecules having coordination number for metal equal to 20.