Structural building units of homoleptic coordination compounds

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Abstract

For the known structures of homoleptic coordination compounds, a database of structural building units has been created: complexing atoms, ligands, solvate molecules, and counterions. For each type of structural building units, geometric and topological descriptors were calculated and entered into the knowledge base. Collected information about the structural building units is available through web services hosted at topcryst.com and can be used to design new coordination compounds and predict their properties.

Keywords: homoleptic coordination compound, structural building unit, ligands, complexing atom, solvate molecule, counterion, knowledge base.

Machine learning models that are now widely used can solve complex problems, but this usually requires large datasets that are appropriate for the problem being solved. The higher the reliability of the data and the more complete the sample, the more opportunities are presented for high-quality machine learning and prediction, therefore, at present, data warehouses of a certain content are becoming a popular information product.

In order to fill the repository with users interested in its development, access to data is usually carried out through web services, thanks to which information becomes available from any device connected to the Internet. This format is used in the Cambridge Structural Database (CSD) [1] and the databases of molecules ChemSpider [2] or ZINC [3], the physical properties of materials IRIC [4], the results of quantum mechanical calculations The Materials Project [5], AFLOW [6], Topological Materials Database [7], libraries of topological net types RCSR [8] or Epinet [9].

Volumetric downloads of information calculated from data on crystal structures are of high value for searching for “composition-structure-property” correlations, so we created a database of structural building units (SBU) in crystals of homoleptic coordination compounds (HCC) based on CSD data [1]. Such compounds contain only one chemical sort of ligand with an arbitrary variety of the number

and chemical nature of complexing atoms and outer-sphere particles. Isolation of SBUs from the crystal structure and calculation of their descriptors were performed using the ToposPro software package [10]. As a result, the HCC database we created contains information on 38,595 crystal structures, 60,291 crystallographic sorts of complexing atoms, 18,273 ligands, and 3,253 solvate molecules or counterions. Table contains examples of SBUs for each of the groups.

Table. The first ten leaders in HCC structures of the SBUs, for which the occurrence (N) and share of the total number (ω in %) are given

Metal Atom	N	ω, %	Ligand[&]	N	ω, %	Outer Sphere Particle[&]	N	ω, %
Cu	8137	13.5	Cl_1305	1116	2.87	H_2O_2&O_12	3629	20.43
Ni	5214	8.6	O_12	635	1.63	O_4Cl_1605	1074	6.05
Fe	4344	7.2	Br_1353	524	1.35	C_2H_3N_1318&C_2N_39124	498	2.80
Zn	3627	6.0	I_1320	514	1.32	Cl_1305	439	2.47
Ag	3023	5.0	CO_1161	335	0.86	F_6P_8497	421	2.37
Co	2974	4.9	CHO_2_1	221	0.57	NO_3_1339	378	2.13
Au	2722	4.5	$C_5H_7O_2$_9	215	0.55	BF_4_1808	314	1.77
Li	2089	3.5	CN_1476	171	0.44	CH_2Cl_2_3656	185	1.04
K	1871	3.1	C_5H_5_1429	171	0.44	CO_3F_3S_1453	184	1.04
Pd	1760	2.9	C_2O_4_74	157	0.40	I_1320	183	1.03
Other	*24530*	*40.7*	*Other*	*34831*	*89.6*	*Other*	*10457*	*58.87*

[&]For each SBU, a total formula and a unique number in the database are indicated. Information about water and acetonitrile molecules is combined with their analogs, in which hydrogen atoms are not defined.

The database is accessible through web services https://topcryst.com/index_objects.php and can be useful for searching for regularities in the structure of HCC crystals, as well as for selecting SBUs with suitable chemical and geometric-topological properties in the design and synthesis of new crystalline substances. In addition, the collected data on SSBs make it possible to predict their properties, such as the charge of ligands or the oxidation state of metal atoms, etc. The study was supported by the grant from the Russian Science Foundation № 23-23-00387, https://rscf.ru/project/23-23-00387/

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