Simple Representations of Structural Formulas of Zirconium Compounds

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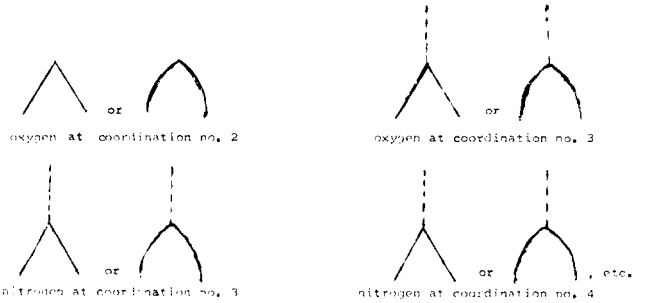
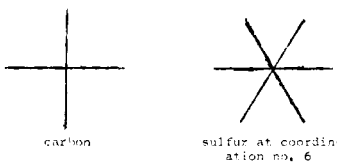
A method is described and demonstrated for the clear graphic representation of structural formulas of simple and complex compounds of zirconium, using solid and broken lines, dots, and small circles. The valency and covalency of zirconium in the particular compound are explicitly revealed, and unused valencies and covalencies, as well as implications of steric effects, are made apparent.

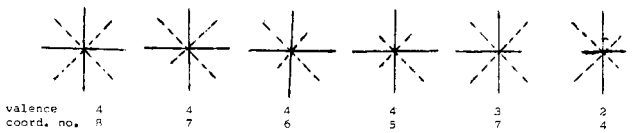
The writer has noted approximately 30,000 articles listed in *Chemical Abstracts* having reference to zirconium and its compounds. A considerable number of these deal with structural formulas of complex molecules. Their graphical representation can be onerous because of the large number of atoms in the molecule or other unit of structure. A simple and unambiguous scheme of representing structural formulas of zirconium compounds is described here, and may serve to reduce the tedium of both writer and reader. The system is but an extension of one introduced over a half century ago by Denison,[1] used by I. W. D. Hackh and Martin L. Grant, and reported by B. R. Siebring at a lecture in 1954, heard by the present author. The extension makes allowance for the variable valence (oxidation number) and coordinate covalency of zirconium, and some structural ramifications not previously depicted in this kind of scheme of presentation.

Basically, the scheme consists in representing an atom of an element by a number of lines emanating from a point. The number of lines is equal to the valency of the element in the specific compound. The lines may be straight or curved, whichever is more convenient, and are regarded as ending at the point of intersection. An apparent extension of a line beyond an intersection is to be considered a different line, not a continuation of a line. The intersection identifies the position of the nucleus of an atom, and the atom, itself. Solid lines generally represent normal covalencies, and broken lines coordinate covalencies. A line representing a valency (valence bond) that is normal for one of the atoms and coordinate for the other may be solid or broken. Further definition is given through examples.

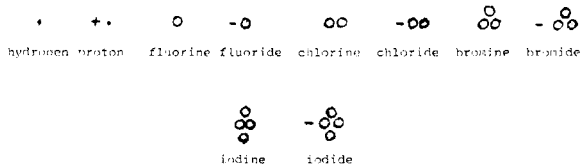




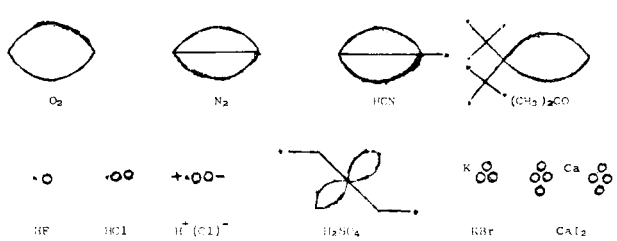
Zirconium almost always has valency (oxidation number) 4 in its compounds, and its coordination number may be any value from 4 to 8. Zirconium will always be represented by the intersection of eight lines, four solid and four broken. Unused valencies will be represented by shortened lines. According to this scheme,



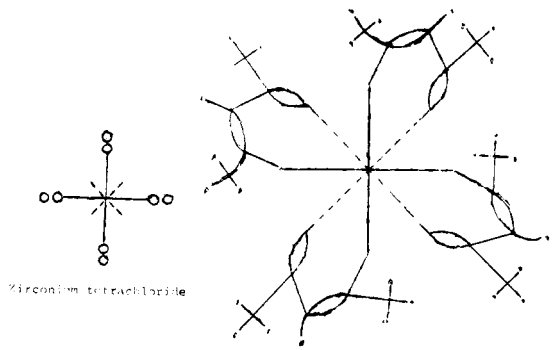
Other metallic elements and ions will be represented by their conventional symbols, except that hydrogen, the proton, and halogens will be represented by a dot, a plus sign and a dot, and small circles.



On the basis of the foregoing, the representations of some compounds other than zirconium compounds would be

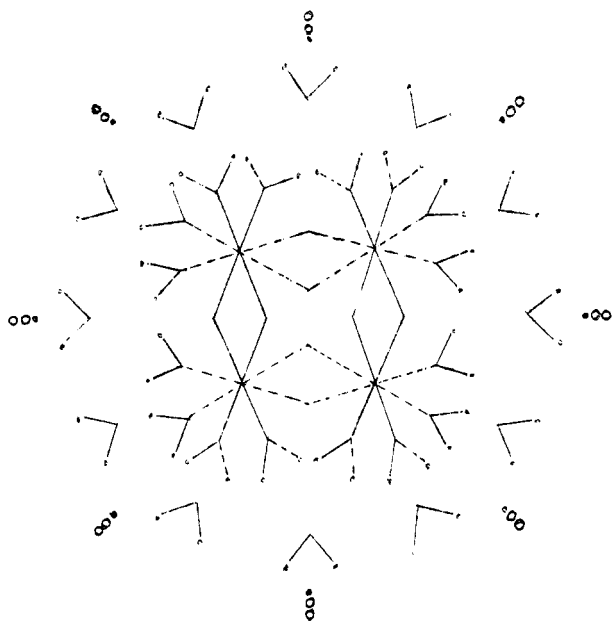


The following examples may now serve to illustrate the representations of structural formulas for a wide variety of zirconium compounds.

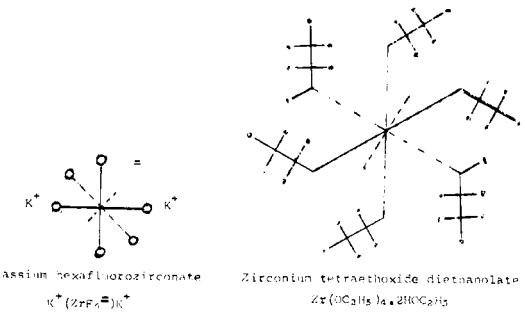


Zirconium tetrachloride

Zirconium tetraacetylacetonate
$Zr(CH_3COCHCOCH_3)_4$

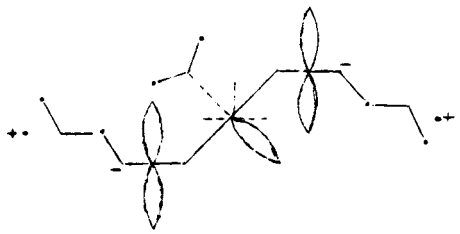


Zirconyl chloride, octahydrate
$(ZrOCl_2.8H_2O)_4$
or
$(ZrO_2.4H_2O.8HCl.12H_2O)$

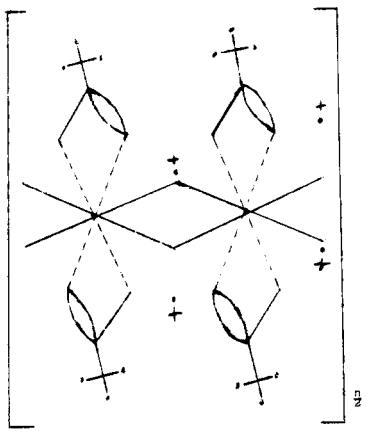


Potassium hexafluorozirconate
$K^+(ZrF_6^=)K^+$

Zirconium tetraethoxide dietnanolate
$Zr(OC_2H_5)_4.2HOC_2H_5$



Disulfatozirconic acid trihydrate
$H_2ZrO(SO_4)_2.3H_2O$



Diacetatozirconic acid
(Zirconium acetate)
$(HZrOOH(C_2H_3O_2)_2)_n$

The chemically uncombined water and hydrogen chloride molecules are placed symmetrically around the chemically bound hydration sphere. Eight lines representing covalent bonds radiate from each of the four centrally located zirconium atoms. Each intersection of two lines, solid or broken, represents an oxygen atom of coordination number 2, and each intersection of two solid lines and a broken line represents an oxygen atom at coordination number 3.

These representations illustrate symmetries and asymmetries of molecules, make the unused valencies conspicuous, and suggest active sites for polymerization or other coordination reactions. They suggest crowding of atoms that might give rise to steric hindrance, repulsions, and related effects.

LITERATURE CITED

(1) Denison, Henry S., *Denver Medical Times* **31**, 360–61 (1912).