

Simple explanation of the experimental ^{57}Fe Mössbauer isomer shift of iron compounds

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According to the existing concept, an increase in electron density on ^{57}Fe nucleus must lead to a decrease in Mössbauer isomer shift (IS). The rise of oxidation state of iron (escape of electrons from the valence shell) usually leads to the decrease in IS, which is explained by the shielding effects.

We suggest applying the approach of the valence shell hybridization to explain the regularities of the IS change [1]. It is easy to show that two electrons on 4s-orbital create the electron density at the iron nucleus, which is equivalent to the density created by the full set of fully filled 4s4p3d-hybridized orbitals:

$$|\psi_s(0)|^2 = \sum_{i=1}^{1+n+m} |\langle \psi_i | \psi_s \rangle|^2,$$

where $n = 0..3$ and $m = 0..5$ are the numbers of the 4p and 3d-orbitals involved in the hybridization. Using this property, we can suggest that the directional chemical bonds, which iron cation establishes with surrounding anions, influence on the IS; this influence being independent on the number of the bonds. Assuming that the IS is proportional to the average bond length, we can explain the observed experimental dependencies. At the same time, d and p-electrons do not create a density on the nucleus. But they affect the ionic radius of the iron ion and, consequently, affect the interatomic distances. Moreover, we concluded that the electron shell of each anion of the iron polyhedron can make noticeable additional contribution to the electron density at the iron nucleus. This makes it possible to explain the dependence of the IS on the iron coordination number.

The speaker is a student or young scientist

No

Section

1. Applications of nuclear methods in science and technology

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