

ROLE OF THE WATER OF CRYSTALLIZATION IN THE MÖSSBAUER  
SPECTRA OF SOME LOW-SPIN FERRIC AND HIGH-SPIN FERROUS  
COMPOUNDS. ITS IMPLICATIONS IN COMPARATIVE STUDIES

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Received 20 March 1995

Accepted 29 March 1995

Mössbauer spectra of low-spin ferric and high-spin ferrous compounds may be sensitive to the local humidity during the measuring process or to other parameters associated with the hydration degree of the sample. This effect is related to the location of water molecules around the  $t_{2g}$  orbitals ( $d_{xy}$ ,  $d_{xz}$ ,  $d_{yz}$ ). The results indicate that for comparative studies all Mössbauer measurements must be carried out in well standardized conditions.

## INTRODUCTION

In a recent paper<sup>1</sup> we have reported on the changes observed in Mössbauer spectra of hexacyanoferrates on dehydration and rehydration. Removing water molecules located in the environment of low-spin  $Fe^{III}$  cations, one can observe notable variations in the quadrupole splitting ( $\Delta$ ) of ferricyanides due to induced changes in the electronic population of the  $t_{2g}$  levels ( $d_{xy}$ ,  $d_{xz}$ ,  $d_{yz}$ ). That first