

# Studies of Dynamics of Hemoglobins by Mößbauer Spectroscopy

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The Lamb Mößbauer factor,  $f'$ , measures the dynamic mean square displacement of a Mößbauer nucleus ( $f' = \exp(-k^2 \langle x^2 \rangle)$ ). Therefore, one can obtain information on the motions within hemoglobin molecules by Mößbauer spectroscopy if one uses the  $^{57}\text{Fe}$  atom of the heme group as a label. The temperature dependence of  $f'$  helps to understand the physical nature of different types of motions.

The study of deoxygenated myoglobin crystals (1) showed that below about 200 K, the Fe vibrates as in other inorganic or organic compounds, and  $\langle x^2 \rangle$  increases linearly with temperature. Above 200 K this increase occurs much faster, indicating that a new channel of motions contributes now additionally. This new channel is attributed to fluctuations of the molecule between different conformational substrates as described by Frauenfelder et al. (2). A similar behaviour was found in Fe of metmyoglobin crystals (3).

In contrast to deoxy myoglobin, the  $\langle x^2 \rangle$ -values of  $^{57}\text{Fe}$  in metmyoglobin show a remarkable anomaly below 170 K: The  $\langle x^2 \rangle$ -values increase with decreasing temperature. This anomaly was also found in oxygenated human hemoglobin molecules (HbA) although absent in deoxygenated HbA. This phenomenon was particularly obvious in partially oxygenated HbA samples, indicating a correlation with the conformations of the molecule. The increase of the mobility of the iron containing part must be balanced by a strong decrease of the mobility of other parts of the molecule.

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1. Parak, F., Finck, P., Kucheida, D. and Mößbauer, R.L., Proceedings of the "V. International Conference on Hyperfine Interactions" Berlin 1980, to be published.
2. Frauenfelder, H., Petsko, G.A. and Tsernaglou, D., (1979) *Nature* **280**, 558 - 563.
3. Parak, F., Frolov, E.N., Mößbauer, R.L. and Goldanskii, V.I. submitted to *J. Mol. Biol.*, reviewed in Parak, F.J. de Phys. (1980) **41**, Coll C1, 71 - 78.