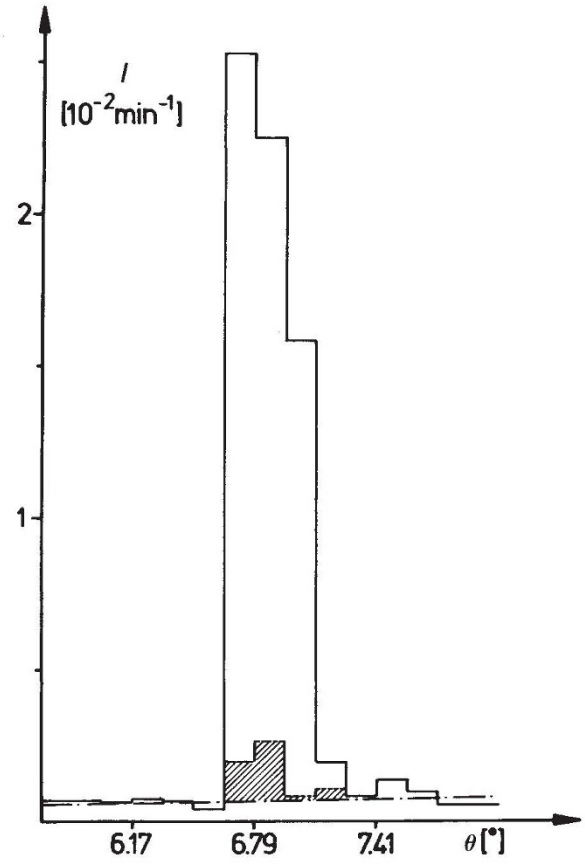

FIG. 2 Bragg reflection 16 2 1 from the myoglobin crystal: solid line, total intensity; hatched area, inelastically scattered intensity at the Bragg positon; dashed-dotted line, correction for Compton effect and smoothly varying diffuse scattering.

The crystallographic B-factor also provides a mean squared displacement, $\langle x^2\rangle^x$, which corresponds to the average deviation of all atoms from their ideal lattice positions. For myoglobin at room temperature a displacement $\langle x^2\rangle^x$ of 0.158 Å^2 has been determined[8]. This value does not include intermolecular motions because the inelastic intensity arising from these modes appears close to the reciprocal lattice node and cannot be separated in the evaluation procedure. The comparison with $\langle x_{1c}^2\rangle$ again shows that motions coupled over short ranges within the molecules are responsible for the main part of the disorder. To determine whether these short-range-coupled displacements are due to static distortions of the molecules or to molecular dynamics, RSMR measurements on a sample containing a large number of small myoglobin single crystals have been made[9]. In this study elastic and inelastic intensities were integrated over spherical shells in reciprocal space, allowing the smoothly varying inelastic component of the thermal diffuse scattering to be included. Although the peaked inelastic component was only 5% of the total integrated intensity of the 16 2 1 reflection (without background), the inelastic scattering at the corresponding resolution of 3.6 Å accounted for 56% of the total intensity in this shell. This large proportion can be explained only if the protein molecules perform intramolecular motions with large amplitudes in accordance with the X-ray results.

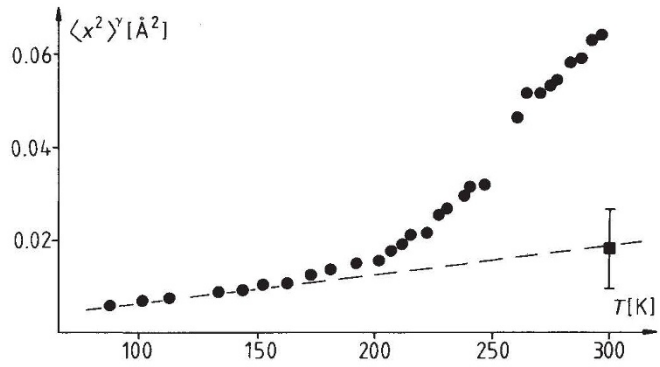

FIG. 3 Mean squared displacements of myoglobin: circles, $\langle x^2\rangle^y$ from Mössbauer absorption experiments[11], square, $\langle x_{1c}^2\rangle$ from the present experiment; dashed line, least squares fit to the low-temperature points. The extrapolation to room temperature gives $\langle x^2\rangle^y = 0.018$ Å^2.

Our experiments constitute the first application of 'Mössbauer crystallography' to proteins. In the future it should be possible to obtain more information by simultaneously exciting many reflections with a divergent beam and collecting the data with an area-sensitive detector. A comparison of diffusely scattered Mössbauer radiation with X-ray scattering should provide insight into the molecular dynamics of many proteins in the crystal state. □

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ERRATUM

Identification of globular mechanochemical heads of kinesin

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AN error in Fig. 1 legend of this letter, in which MgATP was substituted for MgADP, caused the legend to be misleading. A correct explanation is: Kinesin from the Biogel column (lanes 1′, 2′) was incubated with apyrase to hydrolyse contaminating MgATP or MgADP (lanes 3′, 4′). Identical results to those in lanes 1′ and 2′ were obtained in parallel digestion reactions performed in the presence of additional MgADP (1 mM) which yielded identical results to those shown in lanes 5′ and 6′.