Three-dimensional structures of myoglobins reconstituted with synthetic hemes have been determined by means of X-ray diffraction in order to elucidate the functions of heme-proteins. The following four synthetic hemes were used. 

(a) \( R^1 = \text{CH} = \text{CH}_2, R^2 = \text{H} \) 

isopentoheme

(b) \( R^1 = \text{H}, R^2 = -\text{CH} = \text{CH}_2 \) 

pentoheme

(c) \( R^1 = -\text{CH} = \text{CH}_3, R^2 = \text{H} \) 

2-ethyldeuteroheme

(d) \( R^1 = R^2 = \text{H} \) 

4-ethyldeuteroheme 

Crystals of four reconstituted myoglobins, all of which belong to the monoclinic system (space group \( P2_1 \)), are isomorphous with the native myoglobin. Intensity data of (a), (b) and (d) to 2.2Å resolution (ca. 7000 independent reflections) were collected on a FRG four-circle diffractometer. Data collection of (c) is in progress. In Fourier syntheses, phase angles were calculated from atomic coordinates of metMb except for the porphyrin ring (Takano, J. Mol. Biol. (1977) 110, 537).

Electron density map on the heme plane of (a) and (d) are presented in the Figure. In isopentoheme-Mb(a), the modified heme is inserted into apo-Mb in the same position and orientation as that in the native Mb. On the other hand, the heme group is recombined inversely with apo-Mb in 4-ethyldeuteroheme-Mb (d). In pentoheme-Mb(b), most of hemes in crystal locate similarly as those in the native Mb and the rest inversely.

The difference Fourier syntheses \[(P_{\text{modified}}) - (P_{\text{native}})\] do not give any significant peaks except for those of hemes, which show no large change in the main chains and residues in these reconstituted myoglobins.

Figure. left: (a), right: (d)