# *Corrections*

Low-Frequency Dynamics of *Caldariomyces fumago* Chloroperoxidase Probed by Femtosecond Coherence Spectroscopy, by Flaviu Gruia, Dan Ionascu, Minoru Kubo, Xiong Ye, John Dawson, Robert L. Osborne, S. G. Sligar, Ilia Denisov, Aditi Das, T. L. Poulos, James Terner, and Paul M. Champion,*Volume 47, Number 18, May 6, 2008, pages 5156–5167.

Page 5164. The NSD calculations and the results displayed in Figure 12 contain an error. The heme distortion along normal coordinate α was estimated using the scalar product $(\mathbf{X} - \mathbf{X}_0)\cdot\mathbf{Q}_\alpha$ in mass-weighted coordinate space, where $\mathbf{X}$ and $\mathbf{X}_0$ are the mass-weighted atomic coordinates of the input and reference structures, respectively, and $\mathbf{Q}_\alpha$ is the unit vector of the mass-weighted normal coordinate α of the reference (planar ferric porphine). The $\mathbf{X}$ coordinates contain the Fe and 24 porphyrin skeletal atoms. The product $(\mathbf{X} - \mathbf{X}_0)\cdot\mathbf{Q}_\alpha$ is correctly calculated using $\mathbf{M}^{1/2}(\mathbf{x} - \mathbf{x}_0)\cdot\mathbf{M}^{1/2}\mathbf{q}_\alpha/|\mathbf{M}^{1/2}\mathbf{q}_\alpha|$, where $\mathbf{M}$ is a diagonal mass matrix and $(\mathbf{x}, \mathbf{x}_0, \mathbf{q}_\alpha)$ represent atomic coordinates without mass weighting.

The calculation error involved dropping one of the factors of $\mathbf{M}^{1/2}$ in the conversion from non-mass-weighted into mass-weighted coordinates, which significantly reduced the values for displacement given in amu$^{1/2}$ Å.

The corrected version of Figure 12 is shown. Only the six lowest-frequency OOP modes [propellering, ruffling, saddling, waving (*x* and *y*), and doming] are usually considered in the NSD analysis. Here, we also include the inverse doming mode to more accurately model the Fe OOP position, which can be roughly estimated by the sum of doming and inverse doming displacements. This is particularly important if the inverse doming displacement occurs out of phase with the doming displacement (e.g., ferric CYP119).

The discussion of the strong doming coherence observed for CYP101 at 36 cm$^{-1}$ (see Figure 5 and page 5163) should also be modified to indicate that this observation is now consistent with the NSD result.

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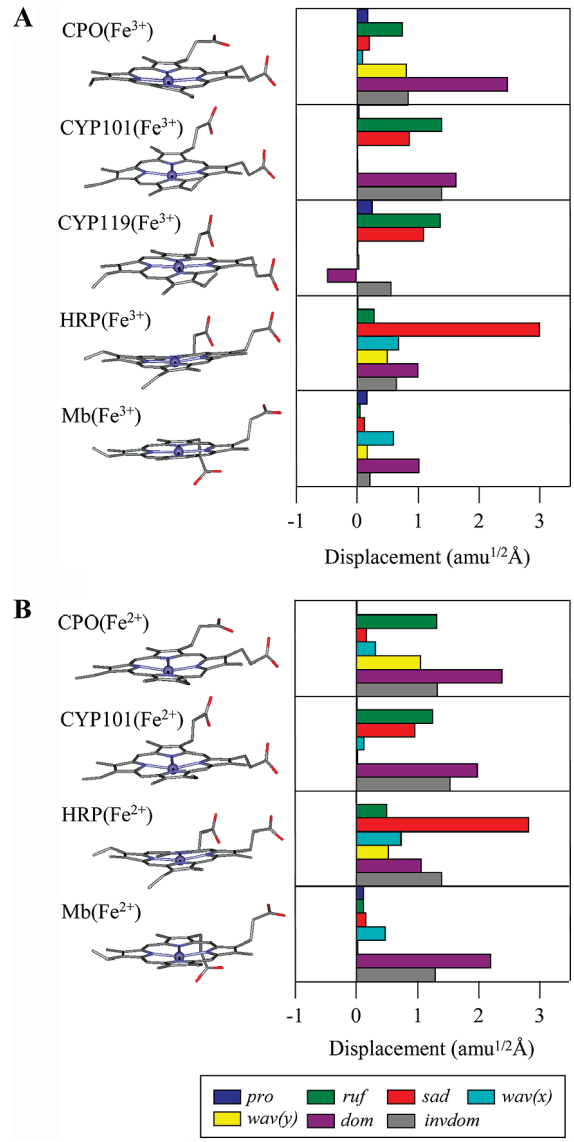


FIGURE 12: NSD analysis in the mass-weighted coordinate space for (A) ferric and (B) ferrous heme proteins (CPO, CYP101, CYP119, HRP, and Mb). The displacement in amu$^{1/2}$ Å is the square root of the sum of squares of the mass-weighted displacements from planarity for Fe and the 24 porphyrin (4 N and 20 C) atoms. The key out-of-plane modes are denoted as follows: *pro*, propellering (blue); *ruf*, ruffling (green); *sad*, saddling (red); *wav(x)*, waving$_x$ (light blue); *wav(y)*, waving$_y$ (yellow); *dom*, doming (purple); and *invdom*, inverse doming (gray). A negative displacement is defined only for doming and inverse doming to indicate the direction of the Fe displacement (+, proximal; −, distal). The PDB entries used to determine the structures are 1CPO, 1DZ4, 1IO9, 1ATJ, 1BZ6, 2J19, 1DZ6, 1H58, and 1BZP for CPO(Fe$^{3+}$), CYP101(Fe$^{3+}$), CYP119(Fe$^{3+}$), HRP(Fe$^{3+}$), Mb(Fe$^{3+}$), CPO(Fe$^{2+}$), CYP101(Fe$^{2+}$), HRP(Fe$^{2+}$), and Mb(Fe$^{2+}$), respectively. The crystal structure for CYP119(Fe$^{2+}$) is not available.