

Multiple-electron excitation in X-ray absorption: a simple generic model. Erratum

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Two typographical errors have been observed in the paper by Roy *et al.* [*J. Synchrotron Rad.* (2001), **8**, 1103–1108]. Equation (16) should read

$$P(\hbar\omega) = P(\infty) \left[\frac{\pi(2n-1)!}{2^{2n}(n-1)!(n+1)!} \right]^{-1} E_B^{n+1/2} \times \int_0^{E_{\max}} \frac{E^{1/2}}{(E_B + E)^{n+2} [1 + t_o^2 (E_B + E)^2]} dE,$$

while the correct form of equation (18) is

$$P(\hbar\omega) = P(\infty) \left[\frac{\pi(2n-1)!}{2^{2n}(n-1)!(n+1)!} \right]^{-1} \times \int_1^{E_p/E_B} \frac{(X-1)^{1/2}}{X^{n+2} [1 + \frac{1}{4}(n-1)^2 (E_B/E_p) X^2]} dX.$$

These typographical errors do not affect our results or conclusions.

References

Roy, M., Lindsay, J. D., Louch, S. & Gurman, S. J. (2001). *J. Synchrotron Rad.* **8**, 1103–1108.

XAFS studies of nitrogenase: the MoFe and VFe proteins and the use of crystallographic coordinates in three-dimensional EXAFS data analysis. Erratum

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One of the authors was omitted in the published version of the paper by Strange *et al.* [*J. Synchrotron Rad.* (2002), **10**, 71–75]. The full author list is given above. Since the acceptance of our paper, an atomic-resolution (1.16 Å) structure of MoFe-protein has emerged [Einsle *et al.* (2002), *Science*, **297**, 1696–1700]. We take this opportunity to update Table 1 of the paper, demonstrating improved agreement of the three-dimensional XAFS refinement with atomic-resolution metrical information.

Table 1

Constrained refinements of the Mo *K*-edge EXAFS using a three-dimensional refinement approach.

In the first refinement, distances are kept at crystallographic values and Debye–Waller (σ^2) values are refined; in the second refinement, the distances are also allowed to vary. A higher value than 0.03 Å² signifies that the atom is incorrectly placed and that little contribution to the EXAFS signal is made. ΔR is the difference in Mo–ligand distance from the crystallographic value averaged over the two independent $\alpha\beta$ units. The final column includes information from a 1.16 Å structure (Einsle *et al.*, 2002).

Ligand	First refinement		Second refinement		ΔR (Å)	1.16 Å structure (Å)
	R (Å)	σ^2 (Å ²)	R (Å)	σ^2 (Å ²)		
Mo–N(His)	2.48	0.11	2.29	0.003	–0.17	2.29
Mo–O5(homocitrate)	2.29	0.11	2.14	0.001	–0.16	2.18
Mo–O7(homocitrate)	2.35	0.11	2.31	0.001	–0.04	2.20
Mo–S1B	2.30	0.001	2.30	0.001	0.0	2.33
Mo–S3B	2.38	0.001	2.37	0.001	–0.01	2.37
Mo–S4B	2.35	0.001	2.35	0.001	0.00	2.33
Mo–Fe7	2.67	0.006	2.67	0.006	0.00	2.67
Mo–Fe6	2.68	0.006	2.67	0.006	–0.01	2.67
Mo–Fe5	2.71	0.006	2.71	0.006	0.00	2.73
Mo–Fe2	5.04	0.01	5.04	0.01	0.00	5.04
Mo–Fe3	5.06	0.01	5.06	0.01	0.00	5.05
Mo–Fe4	5.09	0.01	5.08	0.01	–0.01	5.10
Fit index		12.4		9.5		
<i>R</i> factor	46%		37%			

References

Einsle, O., Tezcan, A., Andrade, S. L. A., Schmid, B., Yoshida, M., Howard, J. B. & Rees, D. C. (2002). *Science*, **297**, 1696–1700.
Strange, R. W., Eady, R. R., Lawson, D. & Hasnain, S. S. (2003). *J. Synchrotron Rad.* **10**, 71–75.