

tions between the coordination numbers and Debye-Waller factors of these two shells, so these parameters are not independent and any change in one will significantly affect the other values on refinement. In this case (where the coordination numbers are known) least squares refinement of the Debye-Waller factors (see Table 1) resulted in a dominant contribution from V-O backscattering. A series of simulations were produced where the total number of oxygen plus sulphur ligands was held at 6 and the O:S ratio varied (only integer values were considered for these coordination numbers and 3 iron neighbours were used throughout); for each ratio, the vanadium-neighbour distances and their associated Debye-Waller factors were refined. This procedure showed that the data could be fitted quite well with 6 oxygen and 3 iron atoms at distances within the limits set above, but the quality of the fit was improved slightly yet significantly by the inclusion of backscattering from sulphur atoms. Consistent with the crystallographic results, the best interpretation of the experimental data (Fig. 2a) required 3 oxygen plus 3 sulphur atoms.

The same approach was adopted in the analysis of the EXAFS data for Ac1* which are shown in Fig. 2b, together with the Fourier transform of the data and the best theoretical fit using the parameters given in Table 2. The EXAFS of Ac1* (Fig. 2b)

Table 2 Parameters used to simulate the EXAFS of Ac1*

Atom	N	R (Å)	$2\sigma^2$ (Å ²)†
O‡	4.0	2.14	0.001
S	2.0	2.32	0.030
Fe	3.0	2.69§	0.014

$E_0 = 17.20$ eV; energy range, 25–398 eV. Error in coordination number considered to be ± 1 ; error in bond distance considered to be ± 0.03 Å.

† Debye-Waller factor.

‡ O, N or C are all possible first shell ligands.

§ Value before correction by addition of 0.05 Å (see text).

resembles that of the VFeS cluster compound (Fig. 2a) and this similarity implies a similar environment for the vanadium. Furthermore, the EXAFS data for Ac1* can be simulated successfully with backscattering contributions from oxygen, sulphur, and iron, the vanadium-neighbour distances being determined as 2.14, 2.32, and 2.69 Å, respectively (all ± 0.03 Å). The V-Fe distance is considered to be ~ 0.05 Å shorter than the true value, given the results for the VFeS cluster compound. As in the interpretation of the EXAFS of this compound, the inclusion of backscattering from oxygen and iron atoms is vital to the quality of the fit and the addition of sulphur atoms significantly improves it. For a total of 6 (oxygen plus sulphur) ligands, consistent with the octahedral coordination deduced from the edge profiles, the best fit was obtained with 4 ± 1 oxygen and 2 ± 1 sulphur atoms. Refinement of the number of iron atom neighbours gave values of between 2.5 and 3.0, for a total of 6 inner shell ligands; these values imply that 3 rather than 2 sulphur atoms are bound to the vanadium.

The major differences in the vanadium K-edge EXAFS of the cluster compound and Ac1* can be accounted for by a reduced Debye-Waller factor and a slightly shorter V-Fe distance in Ac1* (Tables 1 and 2); the former difference suggests a more ordered structure around the vanadium in the protein than in the VFeS cluster compound. The apparent change in the V-Fe interaction (and the possible difference in inner-shell coordination numbers) may account for the differences observed in the XANES region for the VFeS cluster and Ac1* (Fig. 1).

The similarity between the environment of vanadium in Ac1* and of molybdenum in FeMoco⁵ is interesting, suggesting the presence of a vanadium-containing cofactor in Ac1*. By analogy this would include, or form part of, the enzyme's active site. Substitution of vanadium for molybdenum would account for the different substrate specificities of the two nitrogenases¹.

Refinement of the analysis presented above should be possible by extending the range and quality of the data for Ac1* and by studying further model compounds.

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Errata

A protein on *Plasmodium falciparum*-infected erythrocytes functions as a transferrin receptor

Mario H. Rodriguez & Michele Jungery

Nature **324**, 388–391 (1986).

IN this letter Figs 1 and 2 were transposed. The legends are correct as printed.

The essential light chains constitute part of the active site of smooth muscle myosin

Yoh Okamoto, Takamitsu Sekine, Jean Grammer & Ralph G. Yount

Nature **324**, 78–80 (1986).

FIGURES 1 and 2 in this letter were transposed. The legends are correct as printed.

Corrigendum

Searching potential energy surfaces by simulated annealing

L. T. Wille

Nature **324**, 46–48 (1986).

SINCE publication of this letter a sixteen-particle structure has been discovered which is nearly degenerate with that given in Table 1, but has a marginally lower energy ($E = 92.912$). This structure was obtained using exactly the same algorithm and parameters as described in the paper. Due to statistical fluctuations, the five simulations originally reported ended up in the 4^4 configuration ($E = 92.920$), whereas four out of five new runs converged to the new 13^5 structure. It consists of four charges, occupying the vertices of a tetrahedron, and four groups of three charges parallel to each of the faces. This configuration has also been found by J. Edmundson (personal communication) and by Ashby and Brittin (*Am. J. Phys.* **54**, 776; 1986). Interested readers are referred to the unpublished work of Edmundson (May and Baker Ltd, Dagenham, Essex RM10 7XS, UK), who has made an almost exhaustive search of all possible configurations up to $N = 50$. Finally, the Föppl notation for the last entry in Table 1 ($N = 20$) contains a misprint and should read $13^2 6^3 1$.