

neighbouring phosphodiester bonds<sup>1,2</sup>. Other local parameters must therefore also be involved which we are trying to define using a series of DNase I co-crystals with different DNA sequences (G. Frost and D.S., unpublished results).

The H131 residue is essential for the activity of DNase I (ref. 22) and is located at the cut in the complex. We have proposed a mechanism of acid-base catalysis for the nucleophilic attack of a water molecule by the E75-H131 pair<sup>4</sup> (Fig. 3) but definite conclusions cannot be drawn because the scissile bond is cut in solution and is not present in the crystal.

Divalent cations are required for DNA hydrolysis by DNase I (refs 23,24) and we were therefore surprised to find a cut oligonucleotide bound to the enzyme, despite a 1500-fold excess of EDTA over Ca<sup>2+</sup> in the crystallization medium, although the reaction rate was at least 10<sup>4</sup> slower than with cations present. For staphylococcal nuclease the hydrolysis rate was accelerated by Ca<sup>2+</sup> by a calculated factor of at least 10<sup>4.6</sup> (refs. 25). Also surprising was the detection of a second cut in the DNA, induced by diffusion of Mn<sup>2+</sup> into the co-crystals. High pressure liquid chromatography of the dissolved crystals showed that the second cut did occur in the opposite strand, 4 bp away from the first nick (at P307, see Figs 2 and 3). This second site is more than 15 Å away from the first nick and the essential H131, and residues close to the cleaved phosphodiester bond include S40, E13, H41 and D39 (Fig. 3). The contacts to both sites involve the same DNase I molecule and are therefore independent of the crystal packing, so particular environment in the crystal is not responsible for the second cleavage. This indicates that DNase I contains a second, Mn<sup>2+</sup>-activated catalytic site which we are now investigating using Mn<sup>2+</sup>-impregnated DNase I-DNA co-crystals. A second active site could explain reports that DNase I induces double-strand breaks in DNA when activated by Mn<sup>2+</sup> (refs 26-28).

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## Erratum

### Spatial heterogeneity: evolved behaviour or mathematical artefact?

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LINE 4 in the legend to Fig. 1 in this letter should begin "(refs 17-37 and refs listed in ref. 4 as 3, 5, 6, ...)" In the original as printed the reader is referred to ref. 29 rather than ref. 4. □

## Corrigendum

### Synthesis and structure of (cis)-[1-ferrocenyl-2-(4-nitrophenyl)ethylene], an organotransition metal compound with a large second-order optical nonlinearity

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THIS organotransition metal compound was thought to belong to the monoclinic space group Cc. Now the structure has been

re-refined in the orthorhombic space group F2dd, and this is found to be the correct space group using fewer parameters to define the model. In the original paper the crystal data section (Fig. 4 legend) should be replaced as follows:

C<sub>18</sub>H<sub>15</sub>FeNO<sub>2</sub>, *M* = 333.2, orthorhombic, space group F2dd, *a* = 6.015(3), *b* = 44.547(10), *c* = 22.305(6) Å, *U* = 5,976.6 Å<sup>3</sup>, *z* = 16, *D<sub>c</sub>* = 1.48 mg m<sup>-3</sup>, λ(Mo-K<sub>α1</sub>) = 0.70930 Å, μ(Mo K<sub>α1</sub>) = 10.12 cm<sup>-1</sup>, *F*(000) = 2,752. Refinement using full matrix least squares in the new spacegroup resulted in better agreement between observations and model. At convergence *R* = 0.037, *R<sub>w</sub>* = 0.040 for 959 reflections with *I* > 3σ(*I*). Iron, carbons of the cyclopentadienyl ligand (shown to exhibit marked anisotropic vibration), nitrogen and oxygen were refined anisotropically, remaining carbons isotropically and hydrogen in calculated positions, riding on the attached carbon. The cyclopentadienyl rings were refined subject to geometrical restraints.

In the original paper, the views of the molecular packing along the *a* axis and *b* axis were given. The molecular packing remains unaffected by the change of space group and the view along *b* differs from the original figure only by the redefinition of the *c* axis.

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