carboxylate (Fig. 4a). This carboxylate-binding motif is probably involved in binding the C-5 carboxylate of 2-oxoglutarate, the cosubstrate for all known members of the subfamily except IPNS and ACCO, allowing the C-1 carboxylate of 2-oxoglutarate to coordinate to the iron atom[19].

Sequences reported for Fe(II)-dependent extradiol dioxygenases[20–22] display significant sequence similarity to each other, but not to those of the IPNS subfamily. However, crystallographic studies have shown that the coordination chemistry and proposed mechanism of the extradiol dioxygenases share common features with IPNS. The structure of the Fe(III) form of 2,3-dihydroxybiphenyl dioxygenase with a substrate bound reveals two imidazole (His 209 and His 145) and one carboxylate (Glu 260) metal ligands, with the proposed oxygen-binding site *trans* to the glutamate and the substrate ligated directly to the iron[22]. Thus the IPNS subfamily and the extradiol dioxygenases may have convergently evolved similar solutions to the mechanistic problems posed by using dioxygen as an oxidant. □

Methods

Data collection. All data were collected at 100 K using 0.997-Å radiation and a 30-cm MAR research detector (Table 1).

Structure determination of Fe(II):ACV:IPNS. The Fe(II):ACV:IPNS crystals belong to the space group $P2_12_12_1$. Data were processed with the DENZO and SCALEPACK programs[23], and initial phases were calculated by molecular replacement using the program AMoRe[24]. Electron density maps were interpreted using the program O[25]. In 14 cycles of refinement, using the programs XPLOR[26], PROLSQ[27] and SHELXL93 (ref. 28), 328 residues (4–331) were fitted to the electron density. In the final cycle, the positions of all the atoms in the asymmetric unit, including 322 water molecules, a sulphate ion, the ferrous ion and ACV were refined using SHELXL93 which gave a crystallographic *R*-factor of 13.8% (calculated using anisotropic temperature factors).

Structure determination of Fe:NO:ACV:IPNS. Crystals were prepared under anaerobic conditions by transferring a single coverslip with a drop containing Fe(II):ACV:IPNS crystals to a fresh Linbro crystallization tray, injecting NO gas (1 ml) under the coverslip, and rapidly resealing the well. The crystals reacted by diffusion over 1 h and developed an orange–pink colour. Data from these crystals were processed with MOSFILM[29] and the CCP4 suite of programs[30]. An initial structure was obtained by rigid body refinement of the Fe(II):ACV:IPNS main-chain residues into the new unit cell. In 9 cycles of refinement using REFMAC[30], 327 residues (5–331) were fitted to the electron density. In the final cycle, 116 water molecules, iron, NO and ACV were refined. Electron density for the NO was clearly visible throughout the refinement, and the NO was modelled in after two cycles. For both structures, the iron–ligand bond lengths were unrestrained throughout the refinement, and there were no Ramachandran outliers.

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Correspondence and requests for materials should be addressed to J.E.B. or J.H. The crystallographic coordinates have been deposited in the Brookhaven Protein Data Bank (accession nos 1IPS, 2IPS and 3IPS) and will be released one year after publication.

erratum

Photonic crystals: putting a new twist on light

J. D. Joannopoulos, Pierre R. Villeneuve & Shanhui Fan

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Figure 6 in this Review was shown in the wrong orientation. The figure as printed should be rotated 90° anticlockwise. □