**s8a.m7.o5** **Structure of the reduced form of the Iron-only Hydrogenase from *Desulfovibrio desulfuricans* ATCC 7757.** Y. Nicolet[¶], X. Vernede[¶], C.E. Hatchikian[†], J.C. Fontecilla-Camps[¶]. [¶]*Laboratoire de Cristallographie et Cristallogenèse des Protéines, IBS, CEA CNRS, 41, avenue J. Horowitz 38027 Grenoble cedex-France.* [†]*Unité BIP, CNRS, 31 Chemin J. Aiguier, 13402 Marseille cedex France.*

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Hydrogenases are enzymes that catalyze the reversible oxidation of molecular hydrogen according to the following equation: $H_2 <=> 2H^+ + 2e^-$. There are two distinct classes of metalloproteins that are able to catalyze this reaction: the NiFe- and the Fe-only hydrogenases, a classification that is based on their metal content. The former class has been more extensively studied than the latter; the first structure of the NiFe hydrogenase *from Desulfovibrio gigas* was reported in our lab in 1995[1].

Recently, we solved the structure of the Fe-only hydrogenase from *Desulfovibrio desulfuricans* (Dd) to 1.6 Å resolution[2]. In the same time, J.W. Peters and *coll*. solved the structure of the Fe-only hydrogenase I from *Clostridium pasteurianum* to 1.8 Å resolution[3]. A comparison of the active site in the two structures shows some differences most likely due to differences in their redox states. In order to clarify this point it is necessary to study crystals poised at well characterized redox states.

We have recently obtained a fully reduced state of the Dd enzyme that indicates that one of the irons of the active site plays a redox role during catalysis. The structure was solved to 1.85 Å resolution with a very incomplete data set, that required an extensive electron density modification process, in order to calculated interpretable electron density maps. We also have a new evidence for the existence of a specific pathway for $H_2$, from solvent to the active site.

From all these results we conclude that NiFe- and Fe-only hydrogenases constitute a good example of convergent evolution to the same function.

*Notes*

[1] Volbeda A. *et al.* " Crystal structure of the nickel-iron hydrogenase from *Desulfovibrio gigas*", *Nature*, (1995), **373**, 580-587.
[2] Nicolet Y. *et al.* "*Desulfovibrio desulfuricans* iron hydrogenase: the structure shows unusual coordination to an active site Fe binuclear center. ", *Struct. Fold. Des.*, (1999), **7**, 13-23.
[3] Peters J.W. *et al.* " X-ray crystal structure of the Fe-only hydrogenase (CpI) from *Clostridium pasteurianum* to 1.8 Å resolution.", *Science*, (1998), **282**, 1853-1858 (errata: 283, 35; 283, 2102).