Supplementary Material

Theoretical Modeling of the Reaction Mechanism of Phosphate Monoesters Hydrolysis in Alkaline Phosphatase

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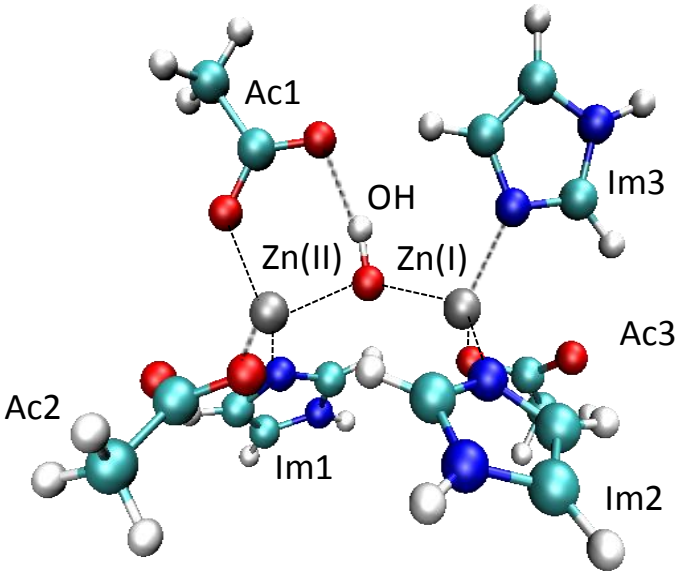

Figure S.1. Gas phase optimized structure for the [Zn(Im)$(Ac)_2$OHZn$(Im)_2$(Ac)] complex (Im stands for the imidazole molecule and Ac for acetate)

Table S.1. Selected interatomic distances between zinc ions and other atoms (in Å) obtained for the [Zn(Im)$(Ac)_2$OHZn$(Im)_2$(Ac)] complex using two different theoretical levels (see text in the paper). Atom numbering refers to figure S.1.

	Zn(I)-Zn(II)	Zn(II)-O_{OH}	Zn(II)-O_{Ac1}	Zn(II)-N_{Im1}	Zn(II)-O_{Ac2}	Zn(I)-O_{OH}	Zn(I)-N_{Im2}	Zn(I)-N_{Im3}	Zn(I)-O_{Ac3}
AM1d-AM1	3.79	2.08	2.09	2.11	2.23	2.01	2.08	2.09	2.09
M05-2X/6-31+G**	3.80	2.00	1.97	2.07	2.07	1.92	2.05	2.06	2.00