

## Efficient catalytic phosphate ester cleavage by binuclear zinc(II) pyrazolate complexes as functional models of metallophosphatases.

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### Streszczenie

A series of dizinc(II) complexes based on the pyrazolate ligands 3-[(1*E*)-*N*-hydroxyethanimidoyl]-4-methyl-1*H*-pyrazole-5-carboxylic acid (**H<sub>3</sub>L<sup>1</sup>**), (1*E*,1'*E*)-1,1'-(4-methyl-1*H*-pyrazole-3,5-diyl)diethanone dihydrazone (**HL<sup>2</sup>**), (*E,E*)-(4-methyl-1*H*-pyrazole-3,5-diyl)bis(methylmethanone) dioxime (**H<sub>3</sub>L<sup>3</sup>**), (*E,E*)-(4-phenyl-1*H*-pyrazole-3,5-diyl)bis(phenylmethanone) dioxime (**H<sub>3</sub>L<sup>4</sup>**), and 1*H*-pyrazole-3,5-dicarboxylic acid (**H<sub>3</sub>L<sup>5</sup>**) have been synthesized and investigated as functional models of phosphoesterases, focusing on correlations between the hydrolytic activity and molecular parameters of the bimetallic core. Speciation of the various dizinc complexes in solution has been determined potentiometrically, and the structures in the solid state have been established by X-ray crystallography. The hydrolysis of two phosphoesters, an RNA model 2-hydroxypropyl-*p*-nitrophenyl phosphate (HPNP) and the pesticide paraoxon-ethyl (POE), promoted by the dinuclear phosphoesterase model complexes has been investigated in DMSO/buffered water (1:1) at 50 °C as a function of complex concentration, substrate concentration, and pH. Drastic differences in the hydrolytic activities of [Zn<sub>2</sub>(**HL<sup>1</sup>**)<sub>2</sub>]<sup>0</sup>, [Zn<sub>2</sub>(**L<sup>2</sup>**)<sub>2</sub>]<sup>2+</sup>, [Zn<sub>2</sub>(**H<sub>2</sub>L<sup>3</sup>**)<sub>2</sub>]<sup>2+</sup>, and [Zn<sub>2</sub>(**HL<sup>5</sup>**)<sub>2</sub>]<sup>2-</sup> are observed and can be attributed to molecular peculiarities. Pyrazolate-bridged dinuclear zinc(II) complexes seem to provide a sufficient number of coordination sites for both activating the substrate and generating the nucleophile, where the phosphate esters are preferentially bound in a bidentate bridging fashion (in the case of HPNP) and in a monodentate fashion (in the case of POE).

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