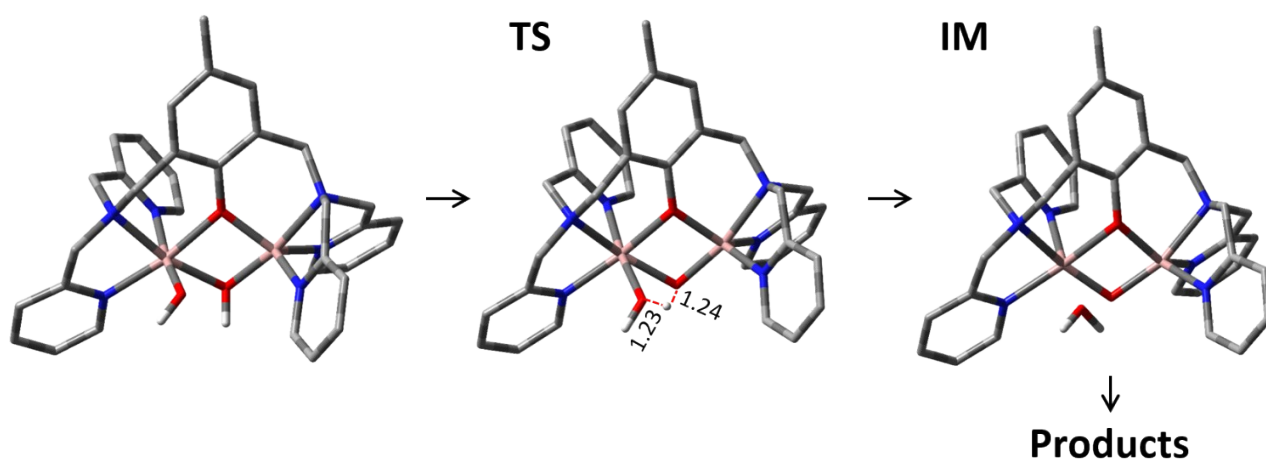
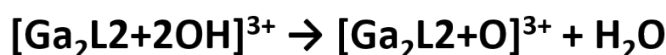


## Influence of the Metals and Ligands in Dinuclear Complexes on Phosphopeptide Sequencing by Electron Transfer Dissociation Tandem Mass Spectrometry

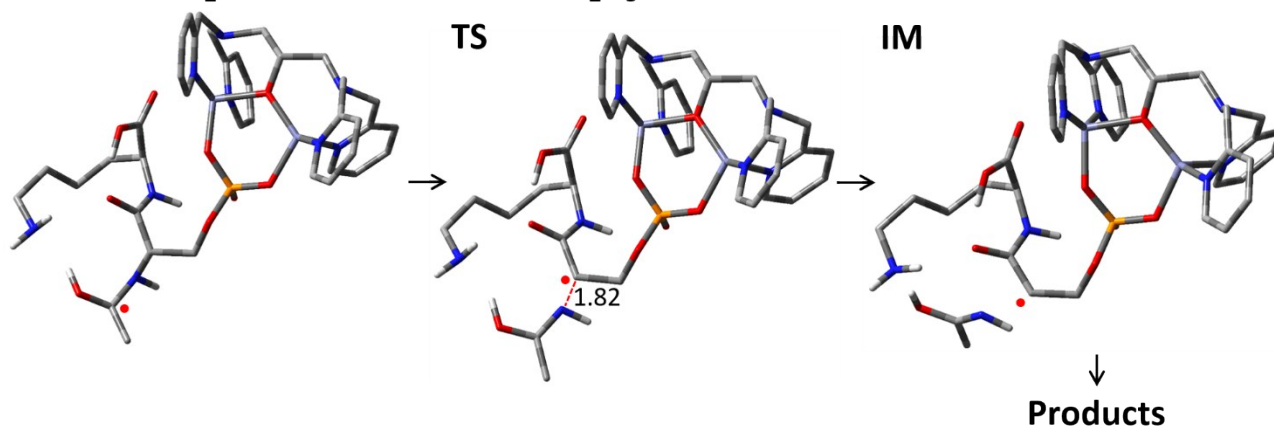
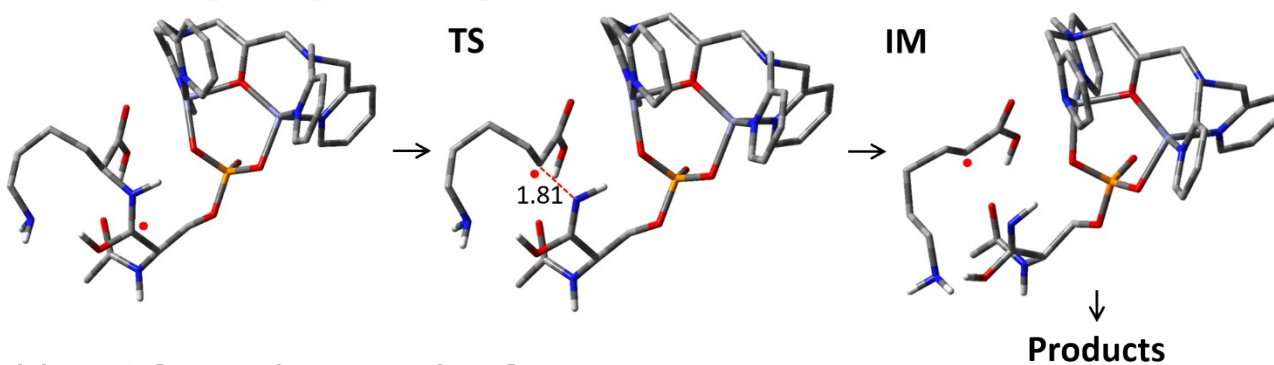
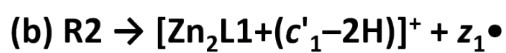
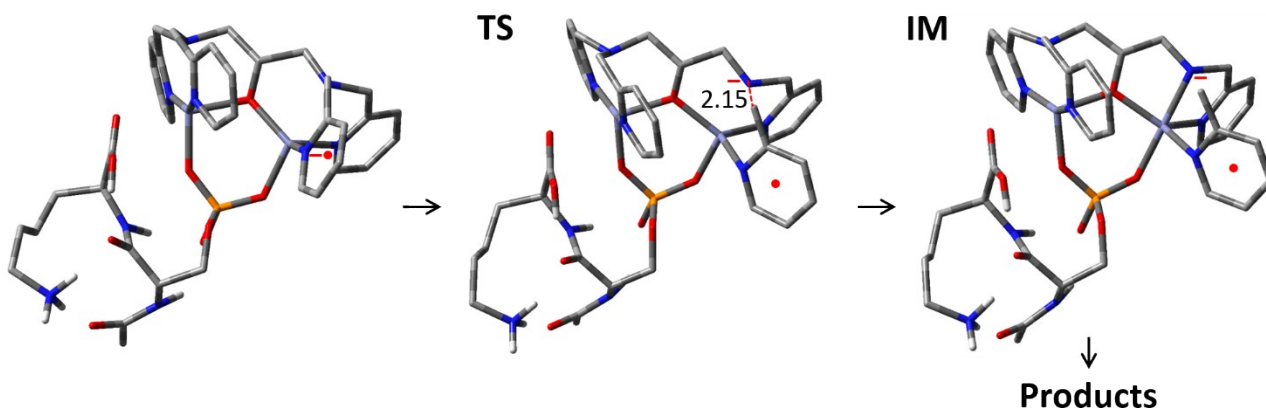
Daiki Asakawa<sup>1\*</sup>, Akio Miyazato<sup>2</sup>, Frédéric Rosu<sup>3</sup> and Valérie Gabelica<sup>4</sup>

1. National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba Central 2, 1-1-1 Umezono, Tsukuba, Ibaraki, Japan
2. Center for Nano Materials and Technology, Japan Advanced Institute of Science and Technology, 1-1 Asahidai, Nomi, Ishikawa, Japan
3. CNRS, INSERM, Univ. Bordeaux, Institut Européen de Chimie et Biologie (IECB, UMS3033, US001), 2 rue Robert Escarpit, 33607 Pessac, France.
4. Univ. Bordeaux, INSERM, CNRS, Laboratoire Acides Nucléiques Régulations Naturelle et Artificielle (ARNA, U1212, UMR5320), IECB, 2 rue Robert Escarpit, 33607 Pessac, France.

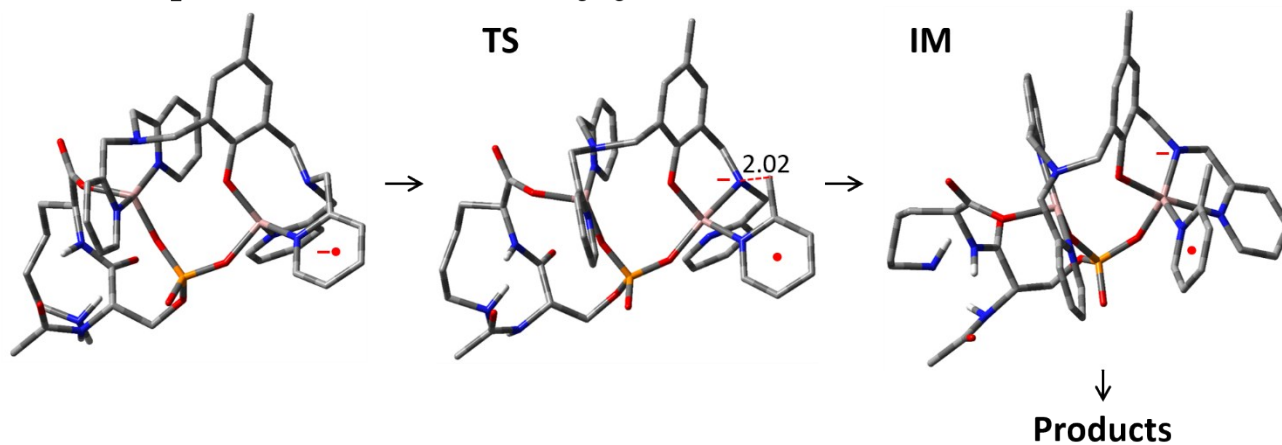
### Supporting Information



**Scheme S1. Mechanism of H<sub>2</sub>O Loss from [Ga<sub>2</sub>L2+2OH]<sup>3+</sup>.** The optimized geometries were obtained by Gaussian 16 with NM16/LanL2DZ/6-31G(d) level of theory. The reaction energies were described in Table 2.



Scheme S2. Mechanism of (a)  $C_6H_6N^\bullet$ , (b)  $z_1^\bullet$  and (c)  $C_2H_5NO$  Loss from  $[Zn_2L1+Ac-pSK-H]^+\bullet$  Cation Radical. The optimized geometries were obtained by Gaussian 16 with NM16/LanL2DZ/6-31G(d) level of theory. The reaction energies were described in Table 3.



Scheme S3. Mechanism of  $\text{C}_6\text{H}_6\text{N}\bullet$  Loss from  $[\text{Ga}_2\text{L2}+(\text{Ac-pSK-3H})]^+$  Cation Radical. The optimized geometries were obtained by Gaussian 16 with NM16/LanL2DZ/6-31G(d) level of theory. The reaction energies were described in Table 4.