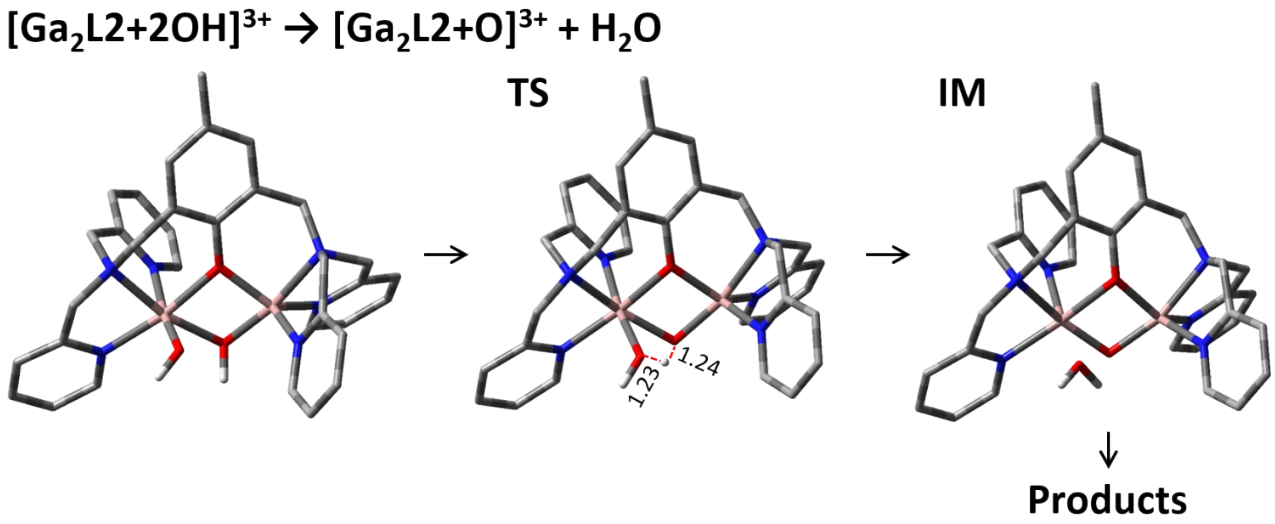
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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

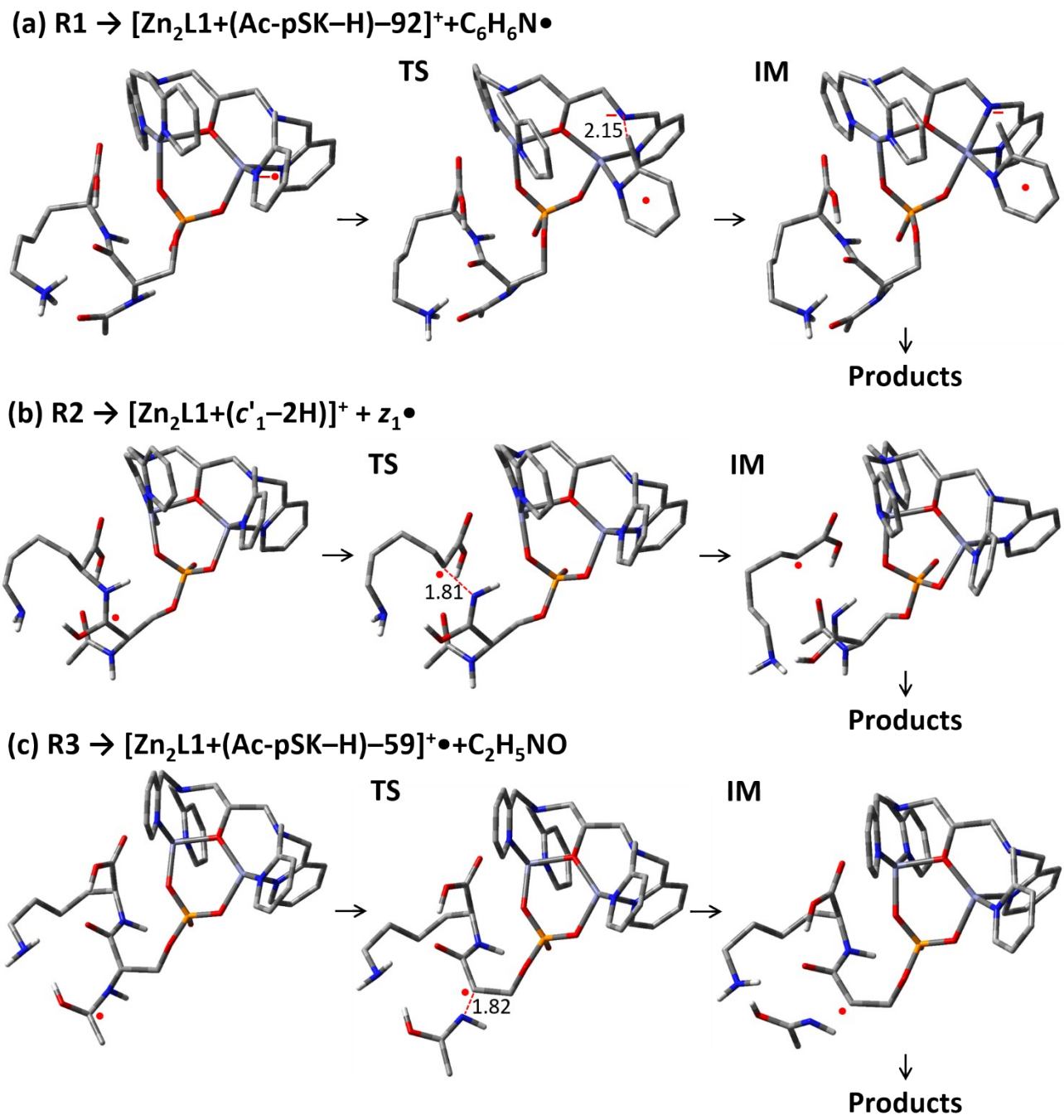
Daiki Asakawa[1*], Akio Miyazato[2], Frédéric Rosu[3] and Valérie Gabelica[4]

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.

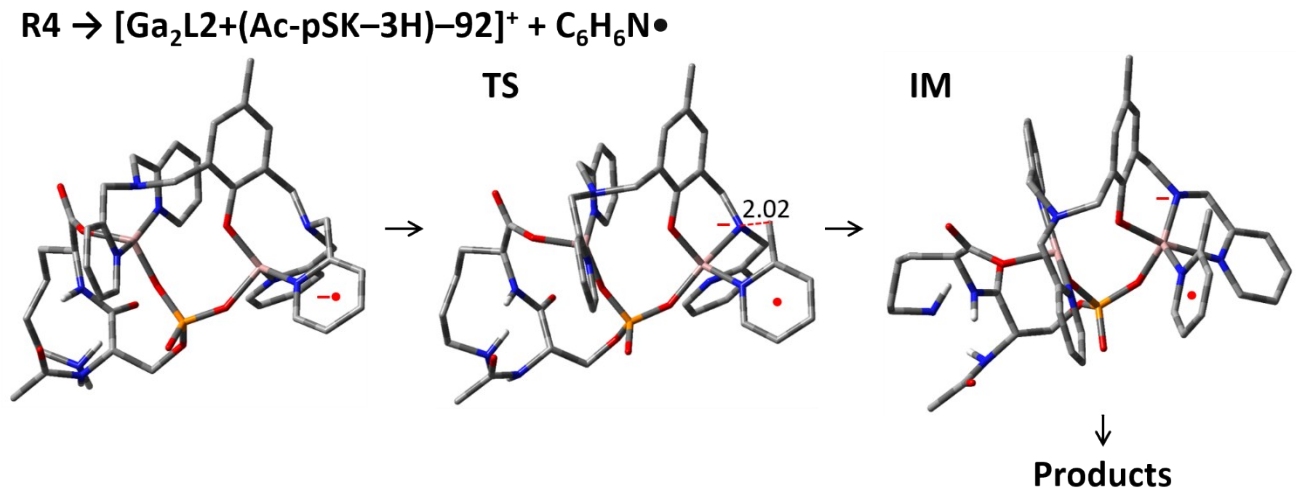
Supporting Information



Scheme S1. Mechanism of H_2O Loss from $[Ga_2L2+2OH]^{3+}$. 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•, (b) z_1• and (c) C_2H_5NO Loss from $[Zn_2L1+Ac\text{-}pSK–H]^+$• 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 C_6H_6N• Loss from $[Ga_2L2+Ac\text{-}pSK–3H]^+$• 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.