

Supporting Information

for

Theoretical studies on the intramolecular cyclization of 2,4,6-*t*-Bu₃C₆H₂P=C: and effects of conjugation between the P=C and aromatic moieties

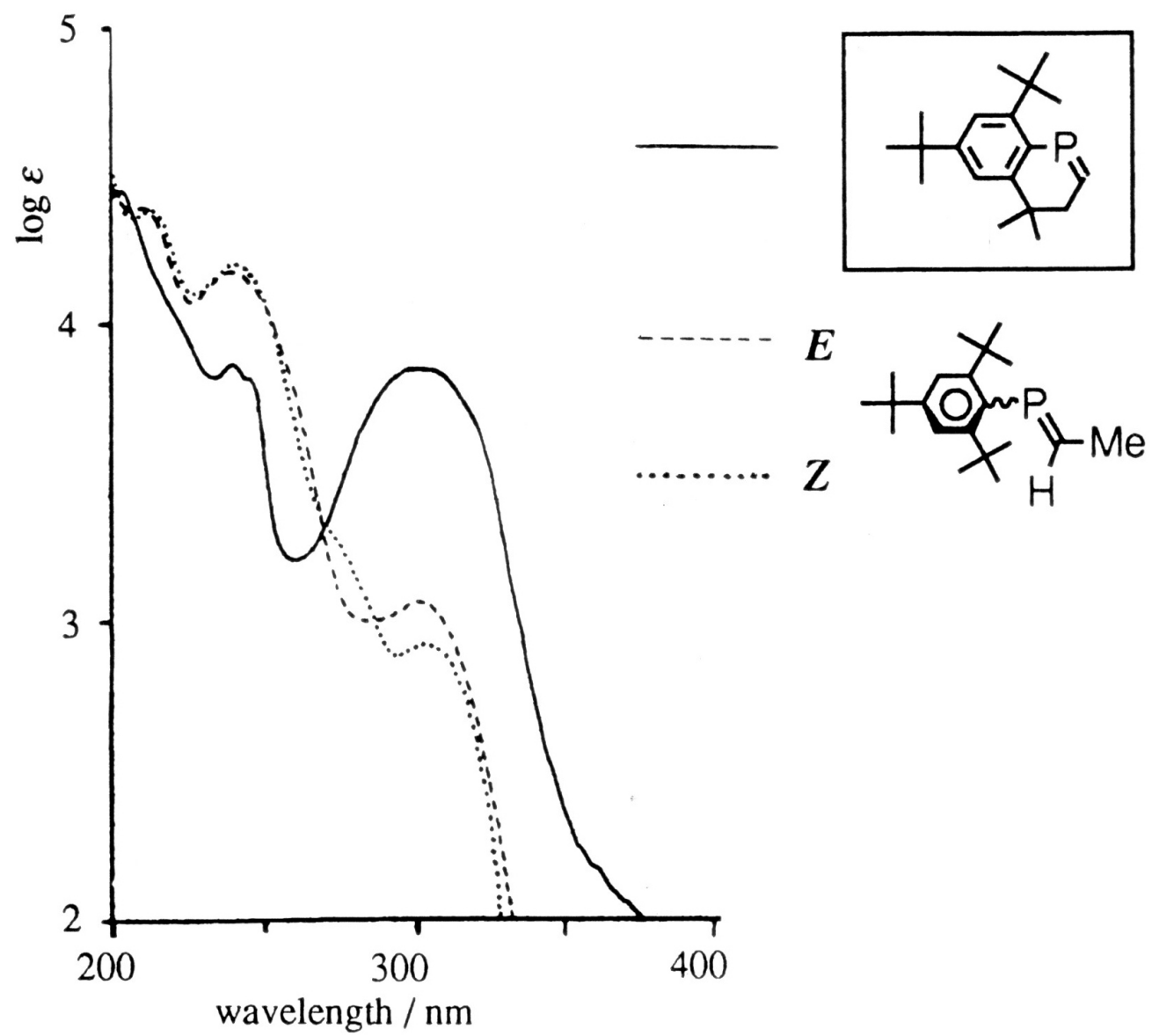
Masaaki Yoshifuji^{1*} and Shigekazu Ito^{1,2}

Address: ¹Department of Chemistry, Graduate School of Science, Tohoku University, Aoba, Sendai 980-8578, Japan and ²Present address: Department of Applied Chemistry, Graduate School of Science and Engineering, Tokyo Institute of Technology, Meguro, Tokyo 152-8552, Japan

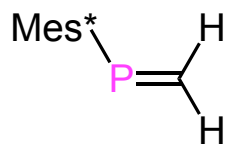
Email: Masaaki Yoshifuji - yoshifj@m.tohoku.ac.jp

* Corresponding author

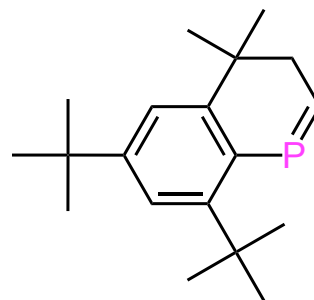
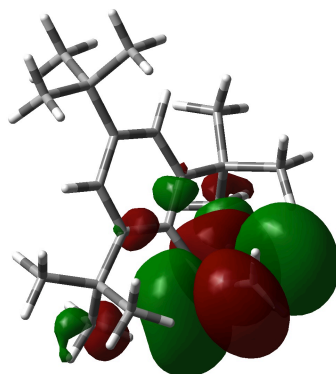
UV Spectra for 2 and Mes*P=C(H)Me and MO for 2 and Mes*P=CH₂



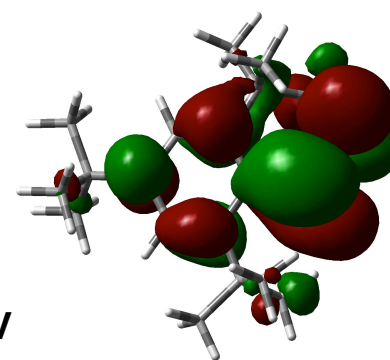
Molecular Orbital: Phosphaalkene



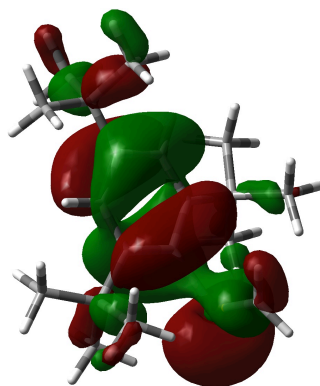
LUMO
-0.180 eV



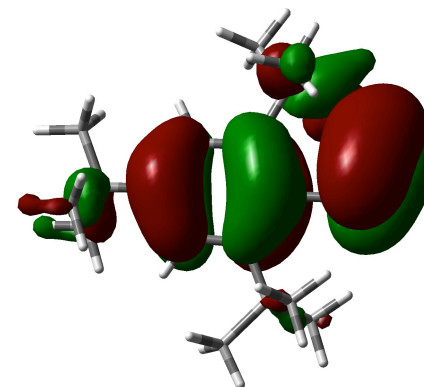
LUMO
-0.422 eV



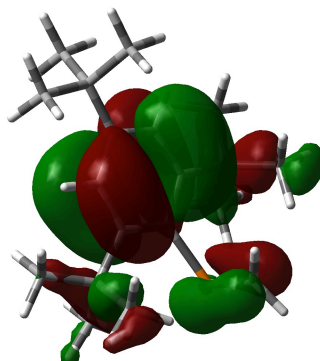
HOMO
-7.64 eV



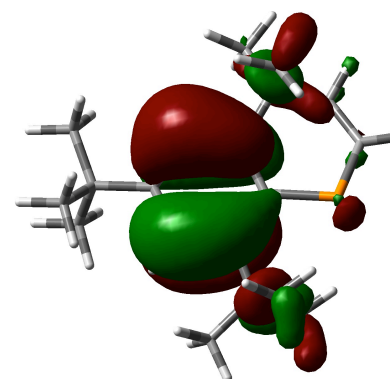
HOMO
-7.34 eV



HOMO-1
-7.95 eV



HOMO-1
-8.01 eV



CAM-B3LYP/DGDZVP