Computational Study on reactivity of cyclic organometallic dienes containing silicon, germanium and tin

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Croatia
Table S1. Total energies of reactants obtained by B3LYP/LANL2DZ (a.u.)

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# Supplementary Material (ESI) for New Journal of Chemistry
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# The Centre National de la Recherche Scientifique, 2006
Table S2. Total energies of transition state structures obtained by B3LYP/LANL2DZ (a.u.)

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-307.400098
### Table S7. Total energies of transition state structures obtained by B3LYP/LANL2DZ* (a.u.)

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*Note: The table contains the energies of transition states (TS) for different pairs of atoms (M, L) and substituents (R) obtained by density functional theory (DFT) calculations using the B3LYP/LANL2DZ* basis set. The energies are given in atomic units (a.u.).*
Table S8. AM1 activation energies in kJmol$^{-1}$

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Table S10. B3LYP/LANL2DZ FMO orbital energies in eV

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I=HOMO(Diene)−LUMO(alkene); II=HOMO(alkene)−LUMO(Diene)

7oxaNBD: HOMO=−6.19, LUMO=−0.95 eV
**Table S11.** B3LYP/LANL2DZ quantum of charge transfer from diene to dienophile\(^a\)

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\(^a\)Negative numbers = electron transfer from diene to dienophile (normal el. demand)
Table S12. Comparison of the length of the forming bond lengths (in Å) in TS1-16 calculated with the B3LYP/LANL2DZ and AM1 methods.

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