

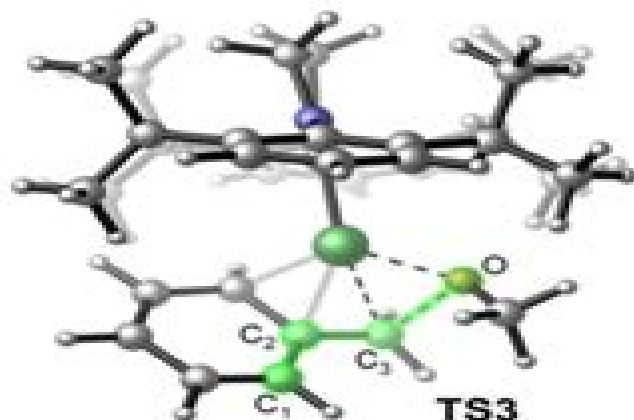
(a) Difference of geometry changes in the absence/presence of AlMe_3



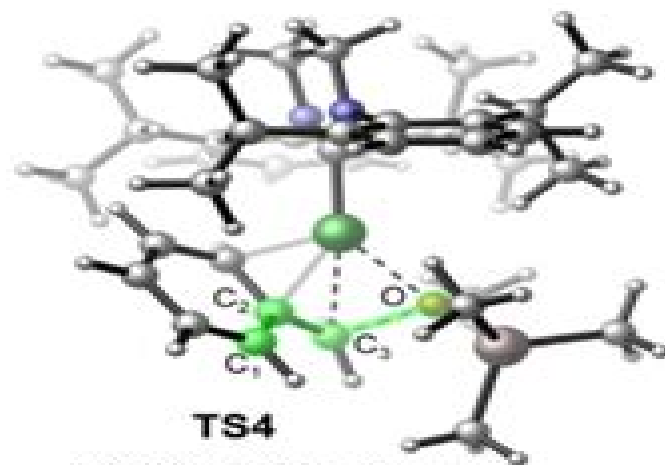
$$D(\text{C}_1\text{C}_2\text{C}_3\text{O}) = 5.8^\circ$$



$$D(\text{C}_1\text{C}_2\text{C}_3\text{O}) = 57.4^\circ$$

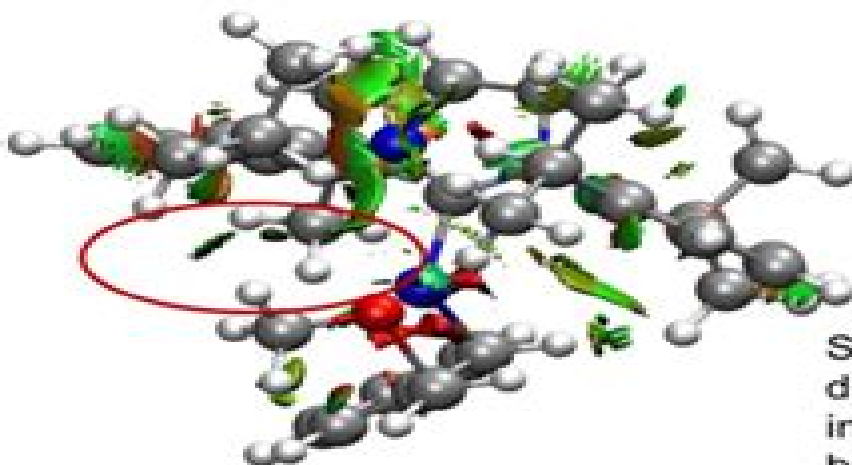


$$D(\text{C}_1\text{C}_2\text{C}_3\text{O}) = 88.0^\circ$$



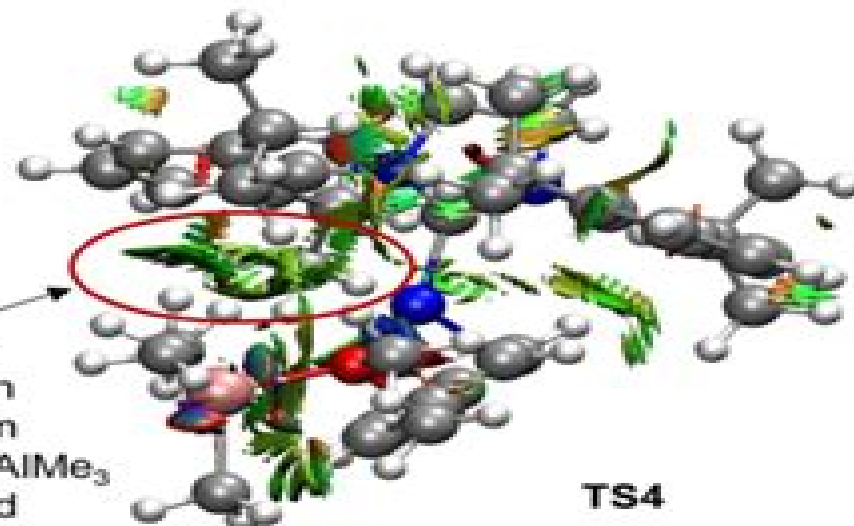
$$D(\text{C}_1\text{C}_2\text{C}_3\text{O}) = 94.2^\circ$$

(b) NCI plots in **TS3** and **TS4**



TS3

Stronger
dispersion
interaction
between AlMe_3
and ligand



TS4

Pg S14 Geometry

Wolfgang Guggemos

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