





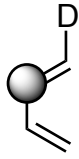
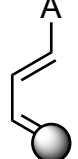
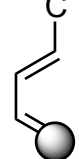
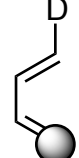
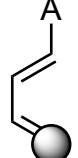
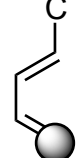
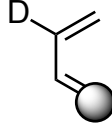
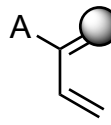
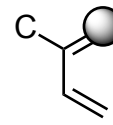
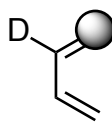
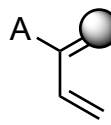
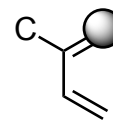
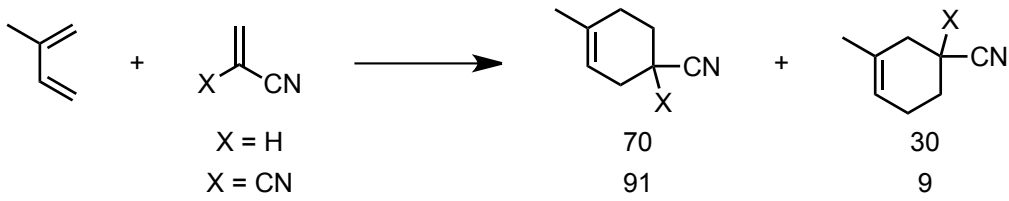


Substituenteneinfluss auf Orientierungselektivität

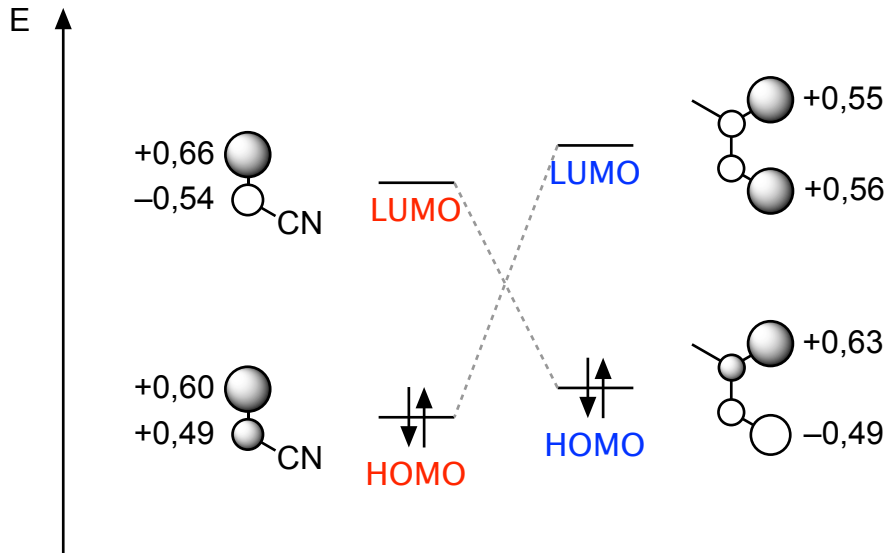
- A Akzeptoren (z.B. $-\text{CO}_2\text{R}$, $-\text{CN}$, $-\text{NO}_2$); erniedrigen die Energien von HOMO und LUMO.
- D Donoren (z.B. $-\text{OR}$, $-\text{NR}_2$, $-\text{CH}_3$); erhöhen die Energien von HOMO und LUMO.
- C in Konjugation stehende Substituenten (z.B. $-\text{Phenyl}$, $-\text{Vinyl}$); erhöhen die Energie von HOMO und erniedrigen die Energie von LUMO.

Position des größten Orbitalkoeffizienten

	D	A	C	
Dienophil				LUMO
				HOMO
1-substituiertes Dien				LUMO
				HOMO
2-substituiertes Dien				LUMO
				HOMO



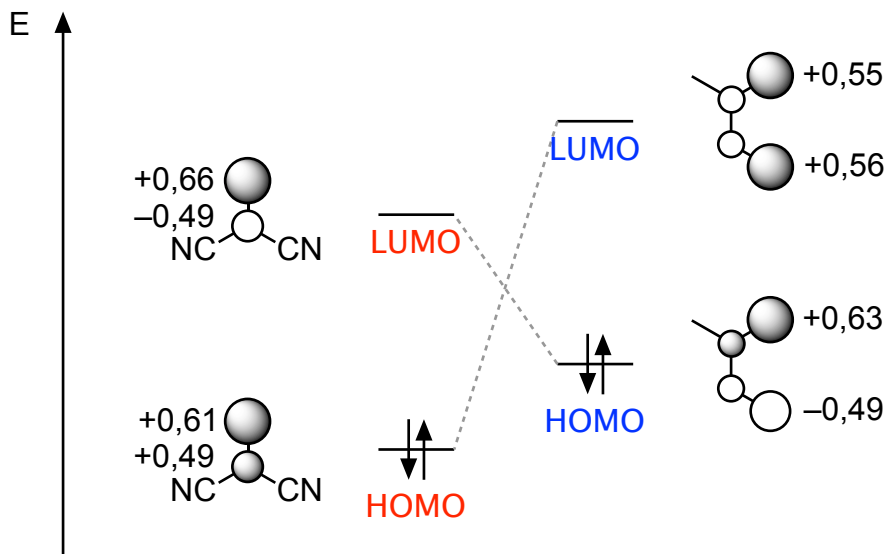
1. Fall: X = H



$$|E_{\text{HOMO}} - E_{\text{LUMO}}| = 11,7 \text{ eV}$$

$$|E_{\text{LUMO}} - E_{\text{HOMO}}| = 8,9 \text{ eV}$$

2. Fall: X = CN



$$|E_{\text{HOMO}} - E_{\text{LUMO}}| = 12,2 \text{ eV}$$

$$|E_{\text{LUMO}} - E_{\text{HOMO}}| = 7,3 \text{ eV}$$