

Organometallchemie

Computermethoden

Table 1 Calculated and experimental M–C bond lengths (Å) for $M(\text{CO})_6$ ($M = \text{Cr}, \text{Mo}$)^a

Method	Cr(CO) ₆ M–C	Mo(CO) ₆ M–C
LDA	1.866	2.035
BP86	1.910	2.077
RPBE ^a	1.925	
B3LYP	1.921	2.068
HF	2.00	
MP2	1.883	2.066
CCSD(T)	1.939	
Exp.	1.918	2.063

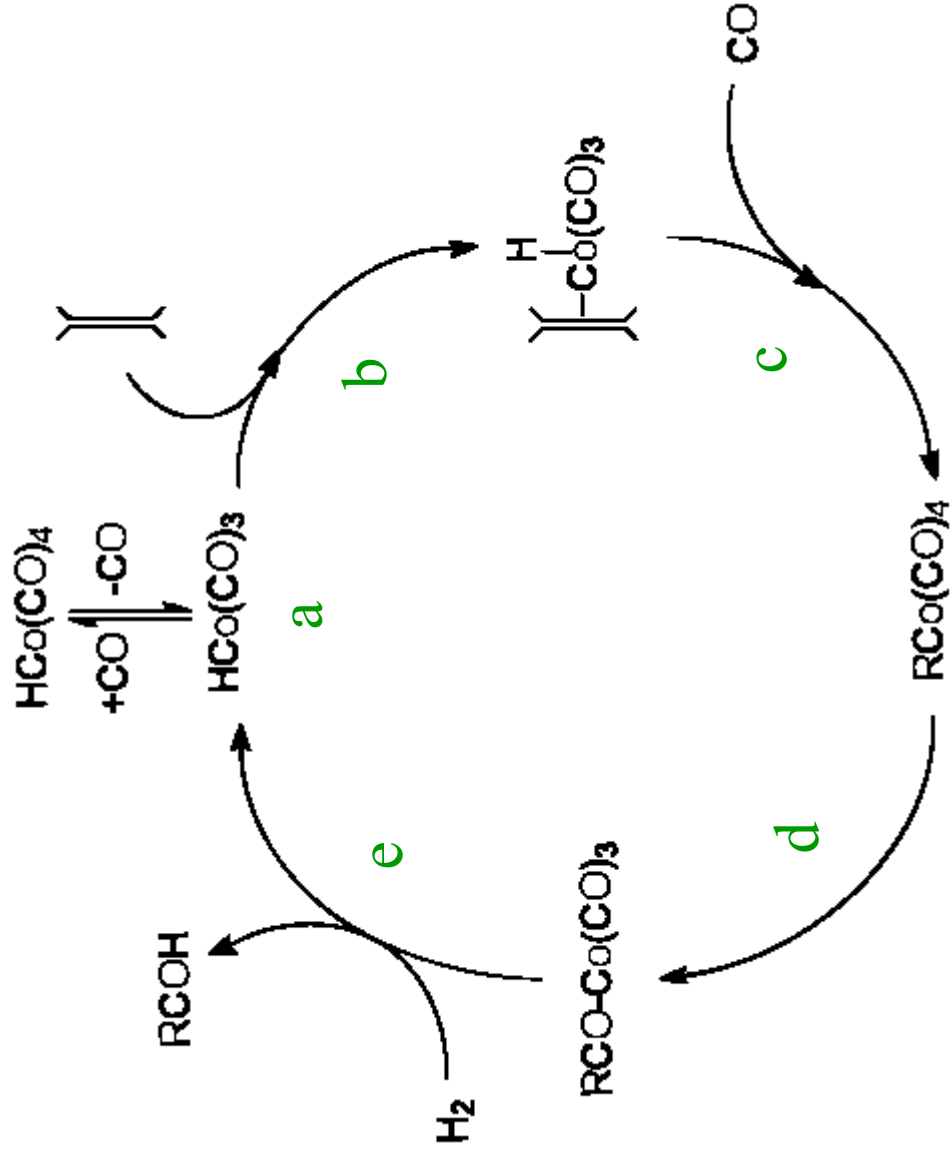
^a All data from ref. 15a except the RPBE results which were taken from ref. 23b.

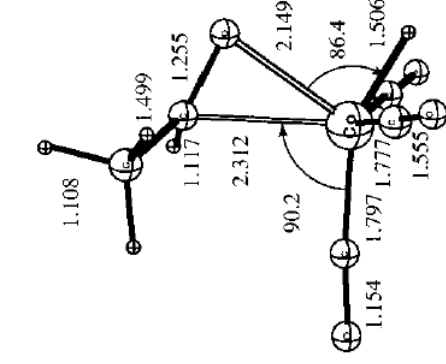
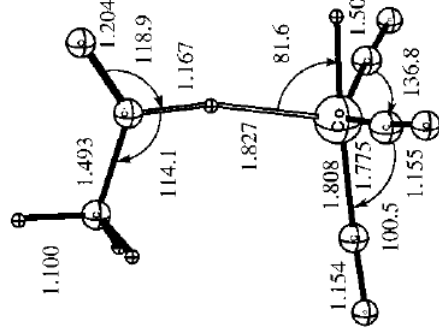
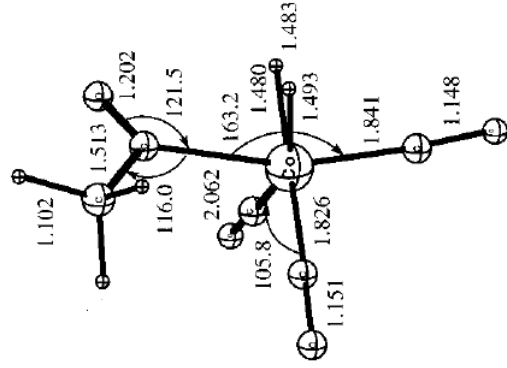
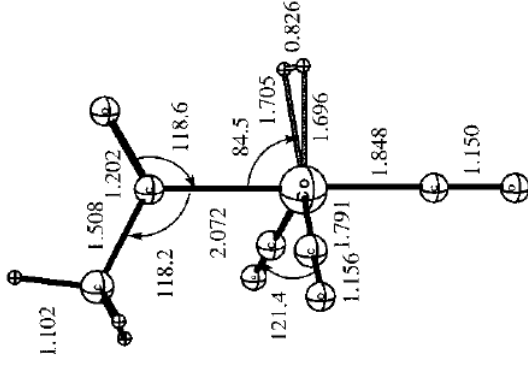
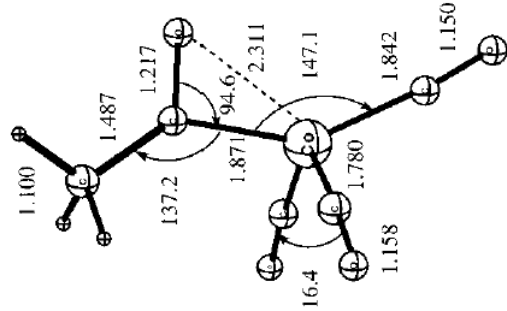
Table 2 First bond dissociation energies (FBDE's) for $\text{Cr}(\text{CO})_6$ and $\text{Mo}(\text{CO})_6^a$

Method	FBDE/kcal mol ⁻¹	
	$\text{Cr}(\text{CO})_6$	$\text{Mo}(\text{CO})_6$
LDA	62.1	52.7
BP86	46.2	39.7
RPBE ^a	36.1	
B3LYP	40.7	40.1
HF	21.0	26.0
MP2	58.0	46.1
CCSD(T)	42.7	40.4
Exp.	36.8 ± 2	40.5 ± 2

^a All data from ref. 9a except the RPBE results which were taken from ref. 23b.

Hydroformylierung - Mechanismus





16c + H₂ (10.5)

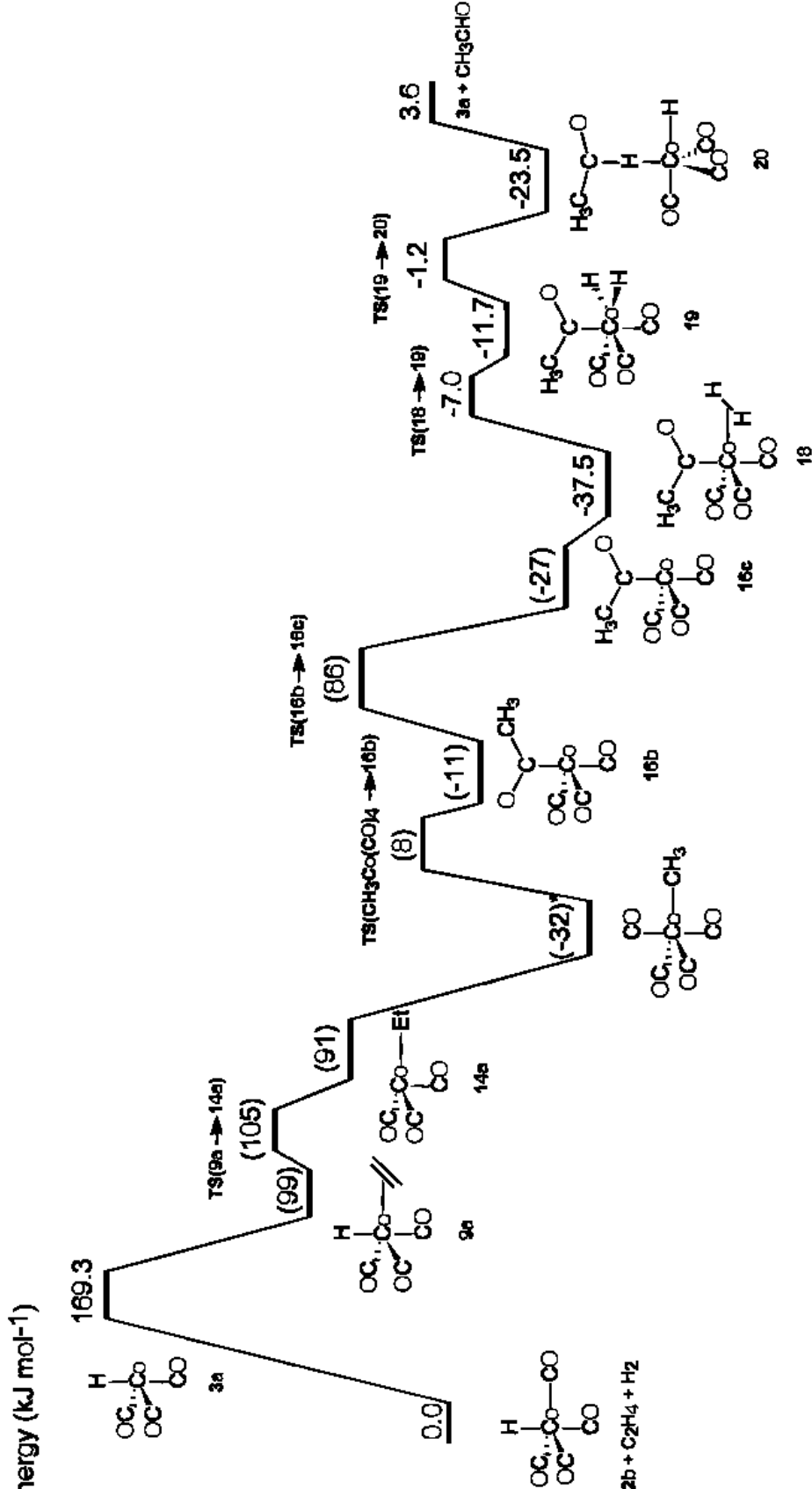
18 (0.0)

19 (25.8)

20 (14.0)

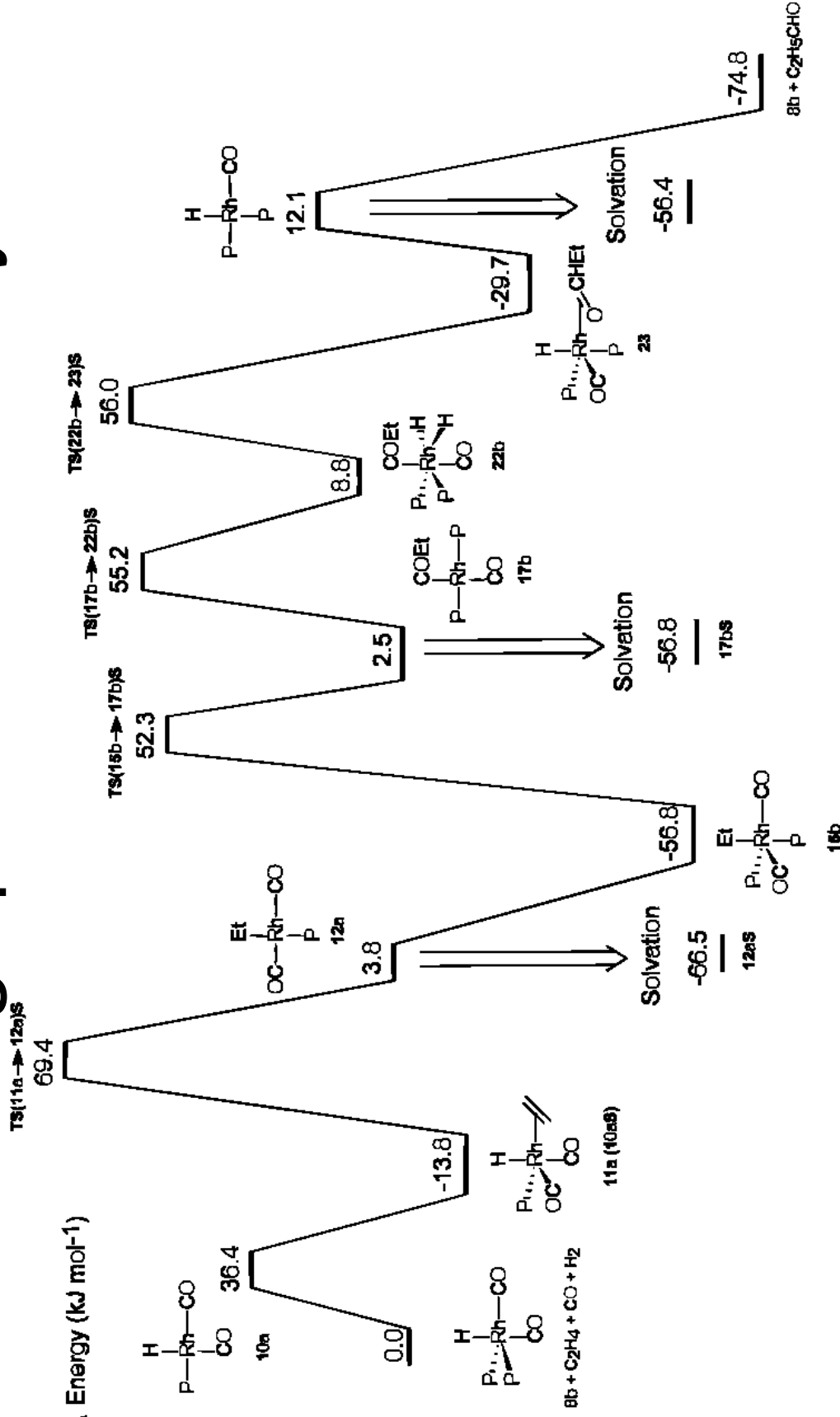
21 (6.1)

Energieprofil – Co-Katalyse



-CO + C₂H₄ C₂H₄ insertion +CO CO insertion H₂ oxidative addition reductive elimination -CH₃CHO

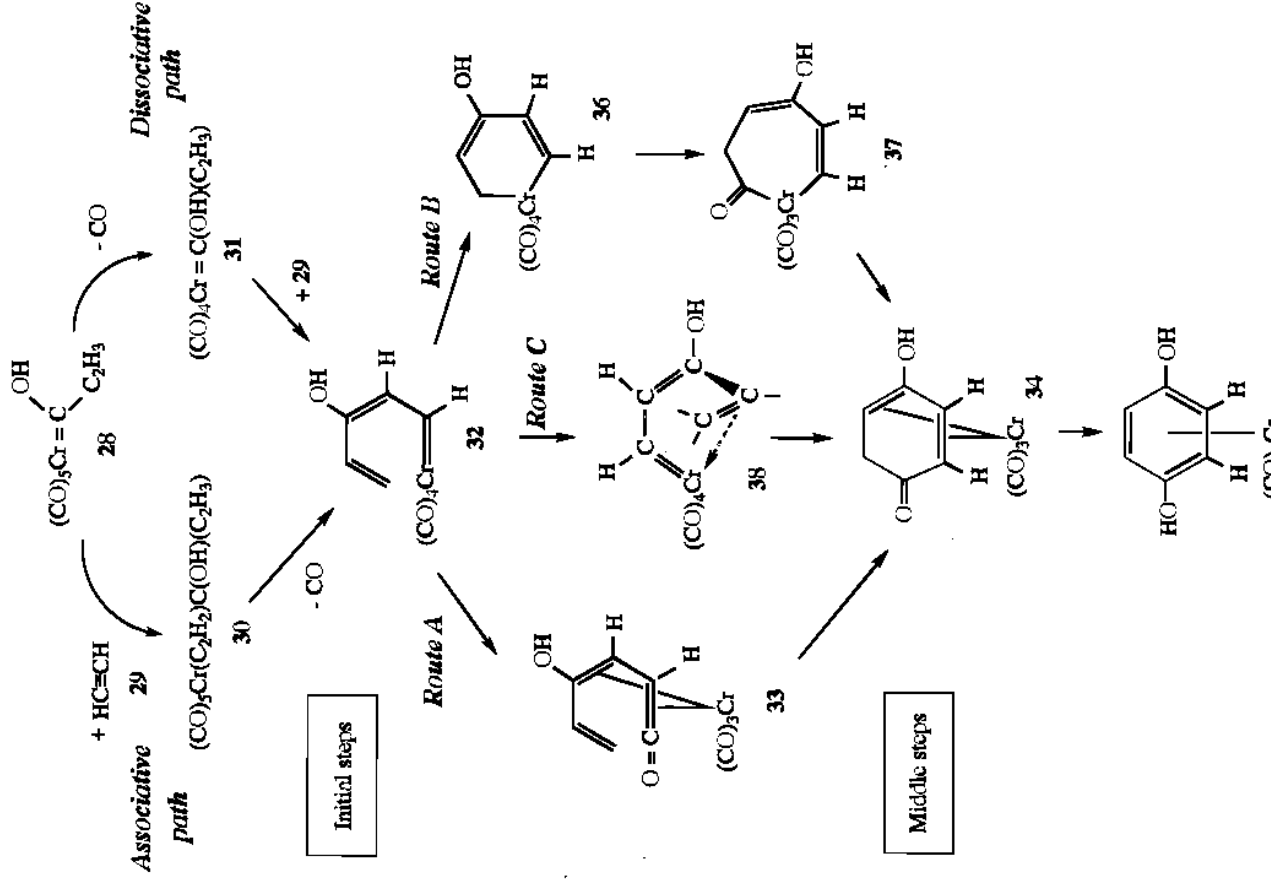
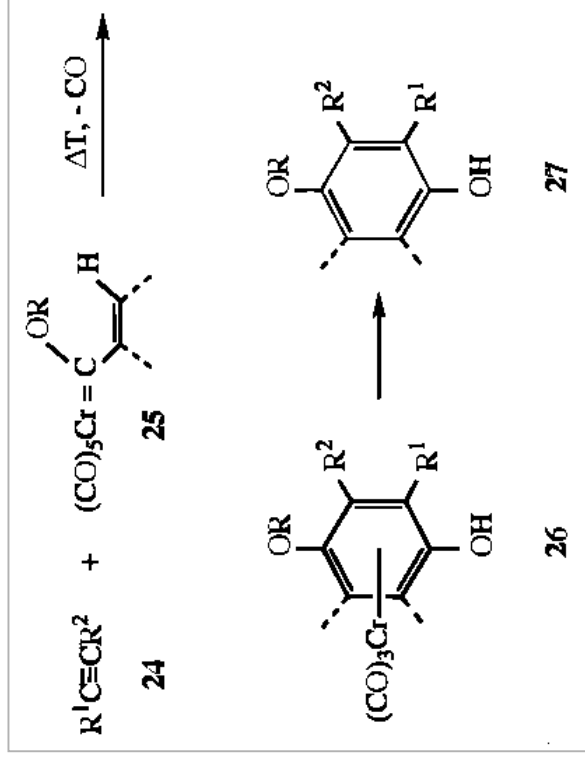
Energieprofil – Rh-Katalyse

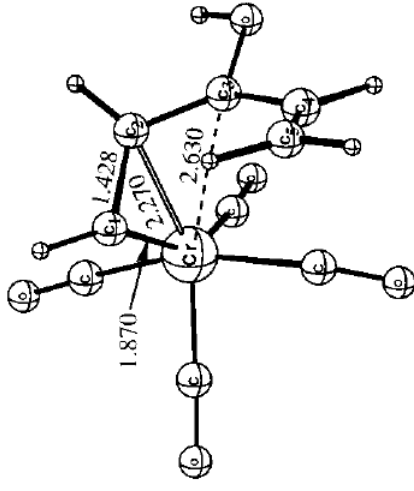
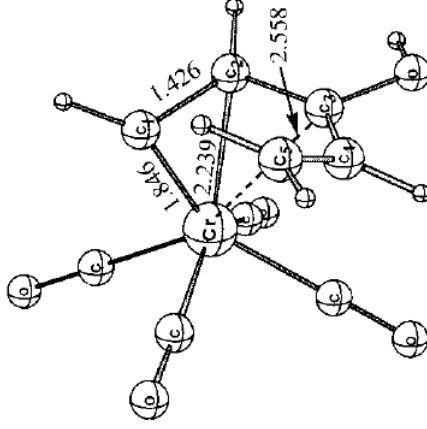
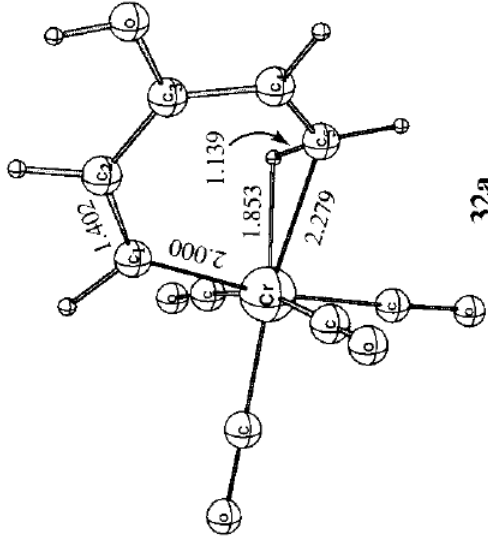


-P + C₂H₄ C₂H₄ insertion +P CO insertion H₂ oxidative reductive -EtCHO +CO

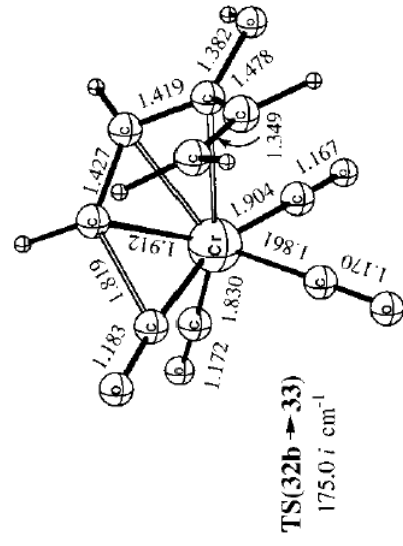
Benzannulierung

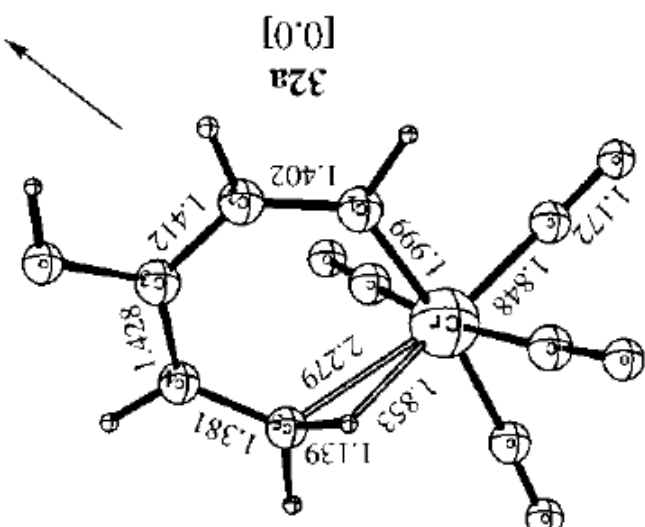
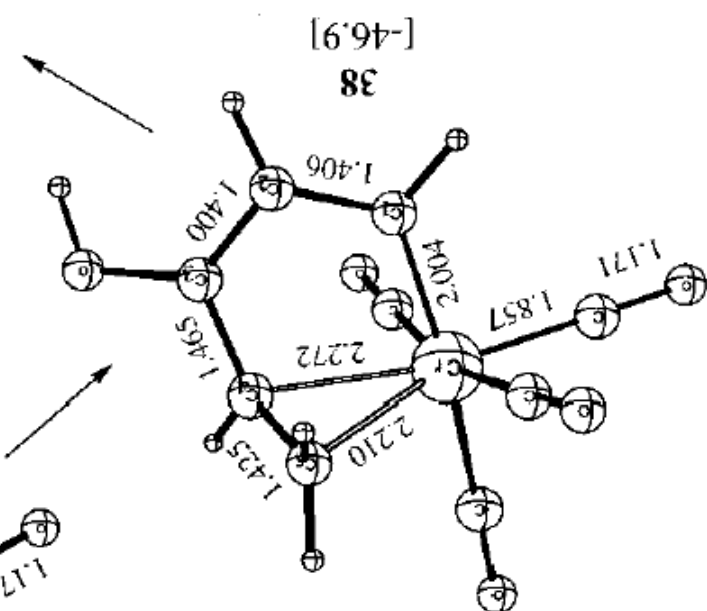
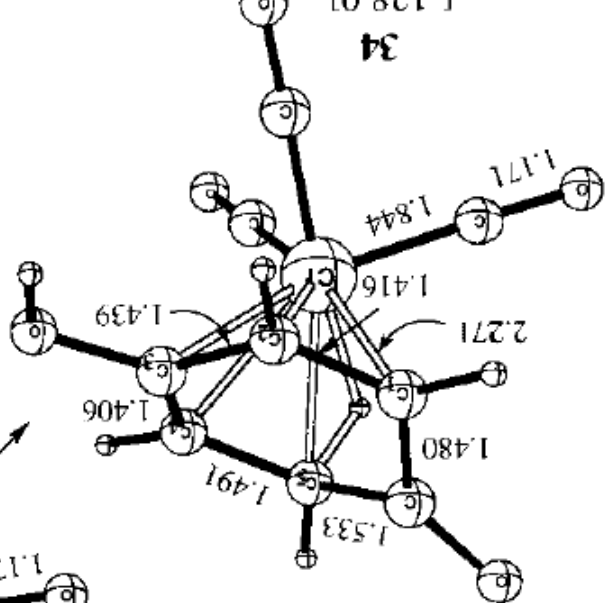
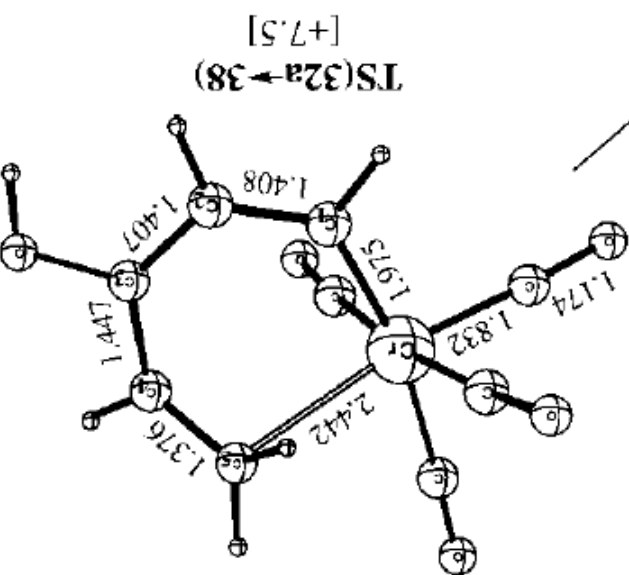
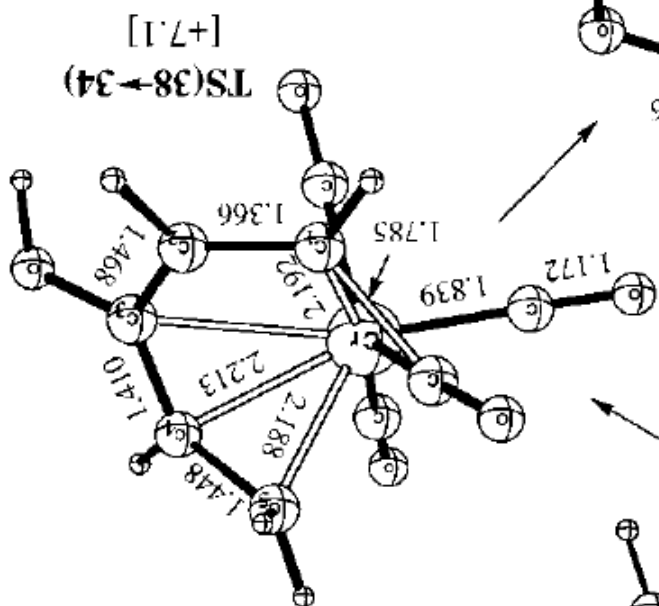
(Dötz-Reaktion)





0.0 kJ mol⁻¹





Energieprofil – Benzannulierung

