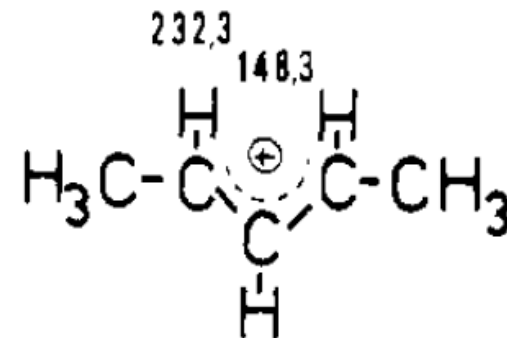
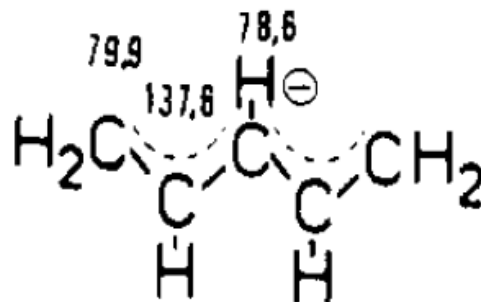
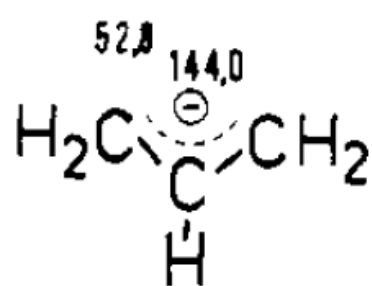
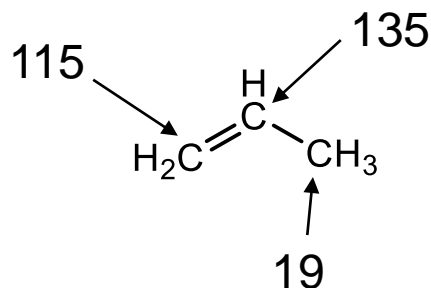


炭素1 mol原子あたりの物質の標準生成ギブズエネルギー (単位kJ)

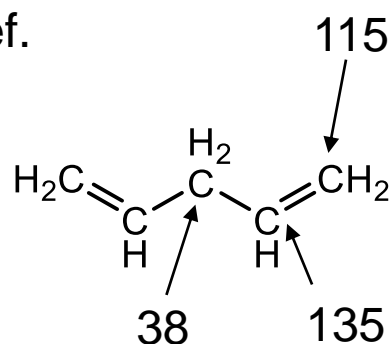
アリルアニオン・アリルカチオンの $^{13}\text{C}$  NMR化学シフト (Me<sub>4</sub>Si基準, ppm)  
 $^{13}\text{C}$  NMR chemical shifts of allyl cation/anions  
 (G. Olah et al., *J. Am. Chem. Soc.*, **100**, 4347 (1978))



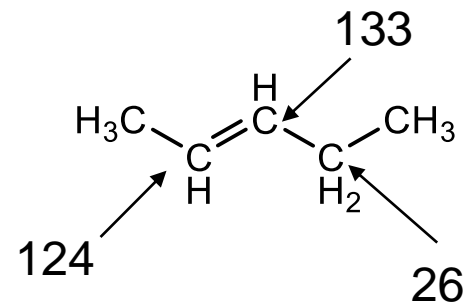
Ref.



Ref.



Ref.

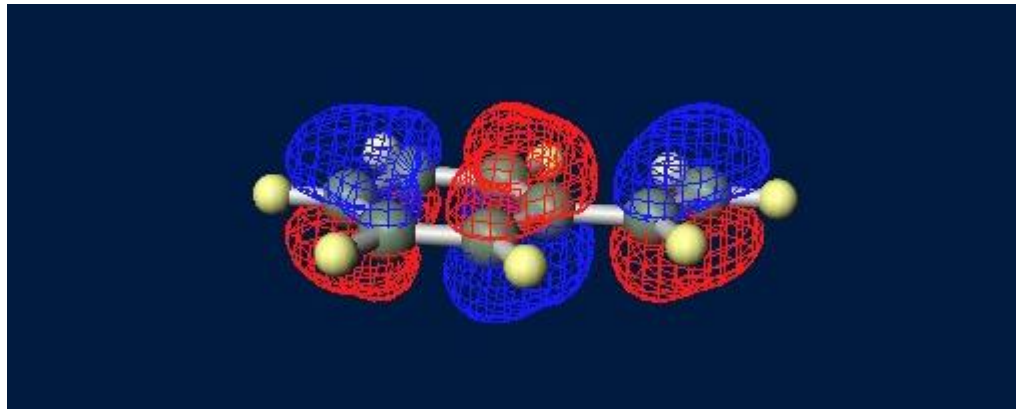


- 両端の等価性, 両端と中心炭素の環境の違い, アニオン・カチオンの化学シフト
- Equivalence of two termini. Difference between terminal and center. Chemical shift of cations/anions

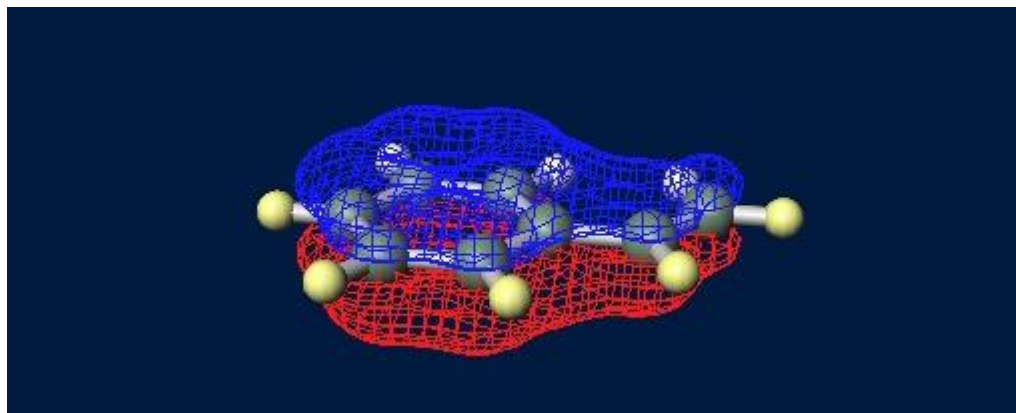
## Molecular orbitals with $\pi$ -character

Styrene  $\text{C}_6\text{H}_5\text{-CH=CH}_2$

HOMO (-9.13 eV)



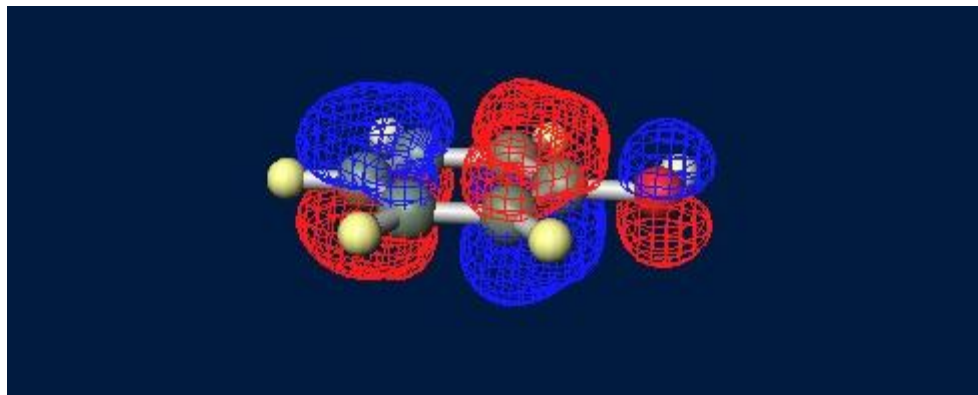
One of other occupied MOs (-13.49 eV)



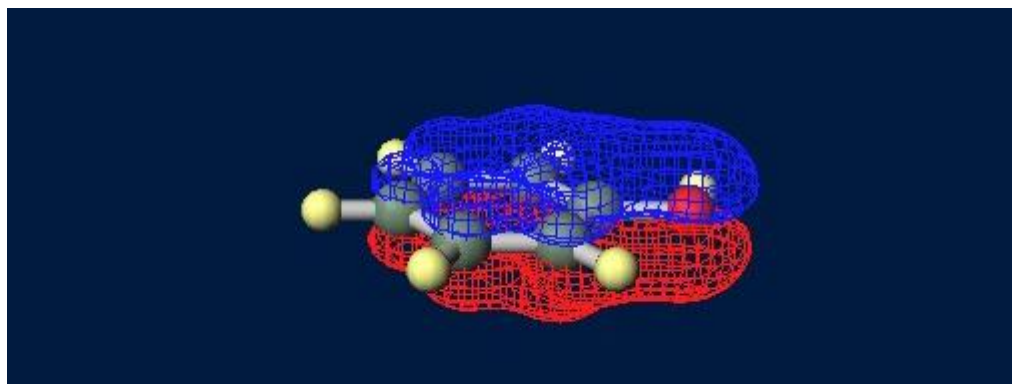
## Molecular orbitals with $\pi$ -character

Phenol  $C_6H_5-OH$

HOMO (-9.17 eV)



One of other occupied MOs (-14.70 eV)

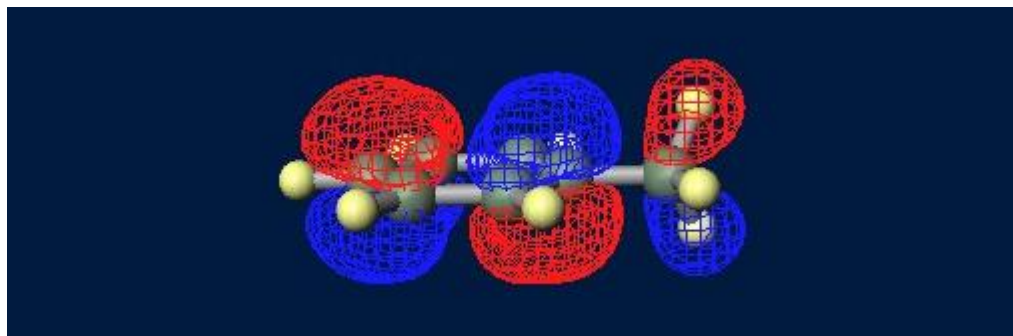


- Oxygen is involved in  $\pi$ -system

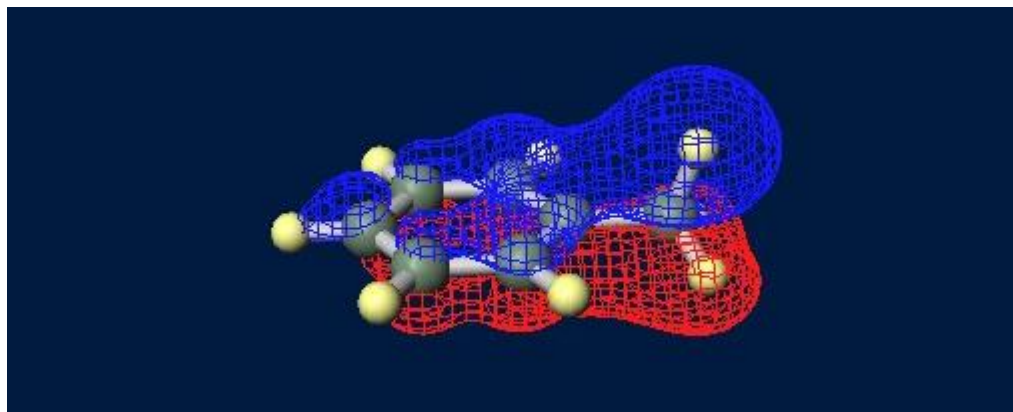
## Molecular orbitals with $\pi$ -character

Toluene  $\text{C}_6\text{H}_5\text{-CH}_3$

HOMO (-9.44 eV)



One of other occupied MOs (-14.57 eV)

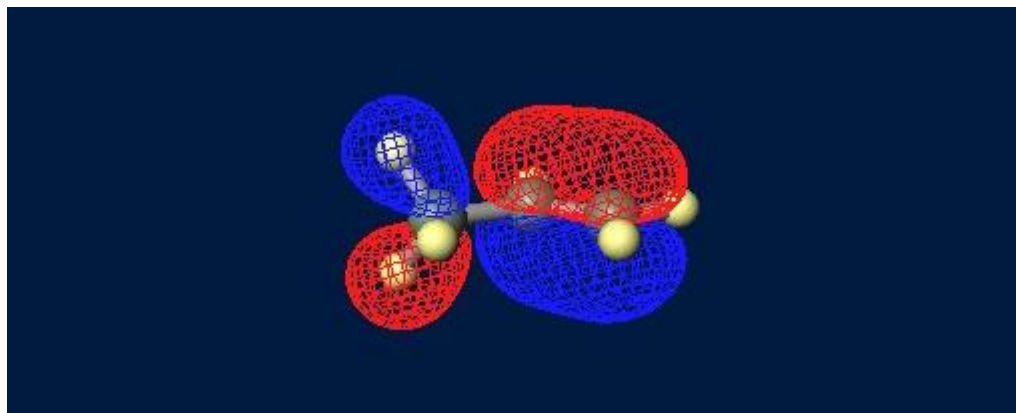


- Methyl group is also involved in  $\pi$ -system !?

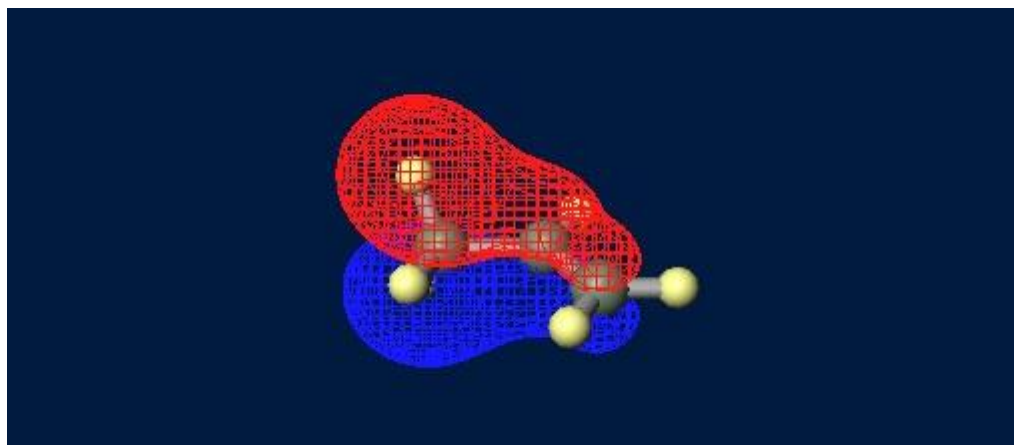
... likewise

propene  $\text{CH}_3\text{-CH=CH}_2$

HOMO (-10.10 eV)



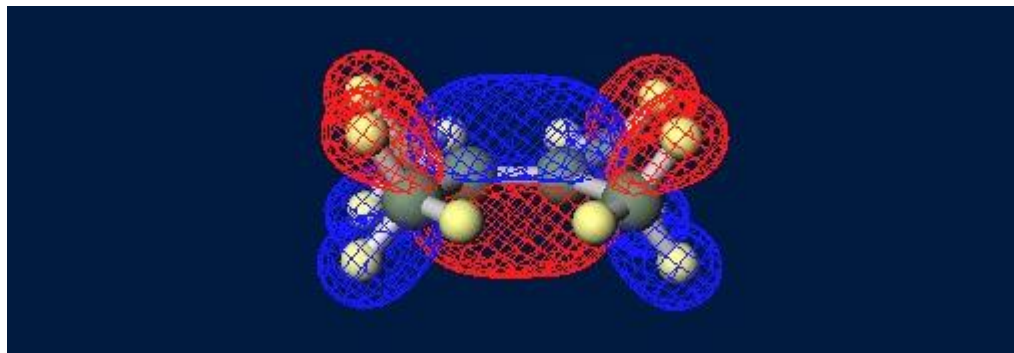
One of other occupied MOs (-14.57 eV)



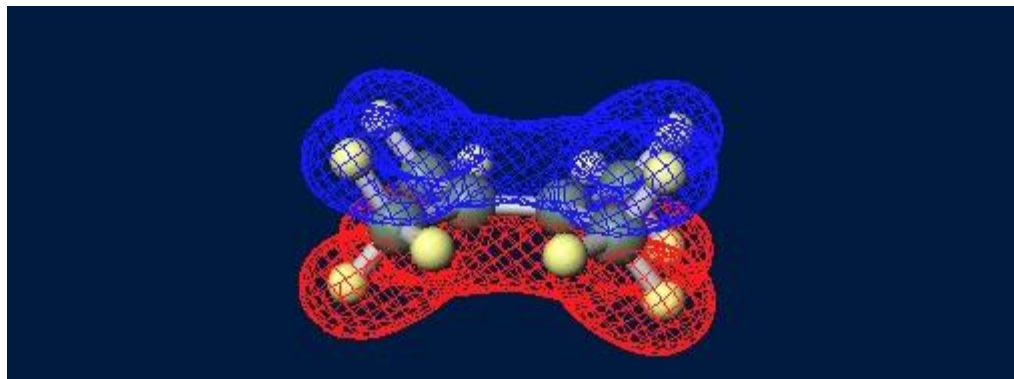
$\pi$ -system is extended to outer alkyl group!

2,3-dimethylbut-2-ene  $(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$

HOMO (-9.14 eV)

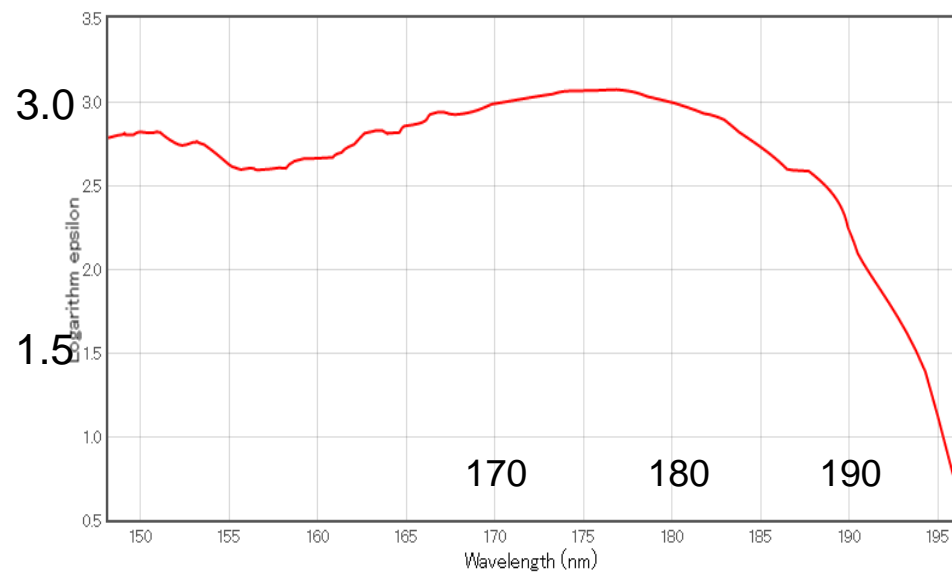


One of other occupied MOs (-15.47 eV)

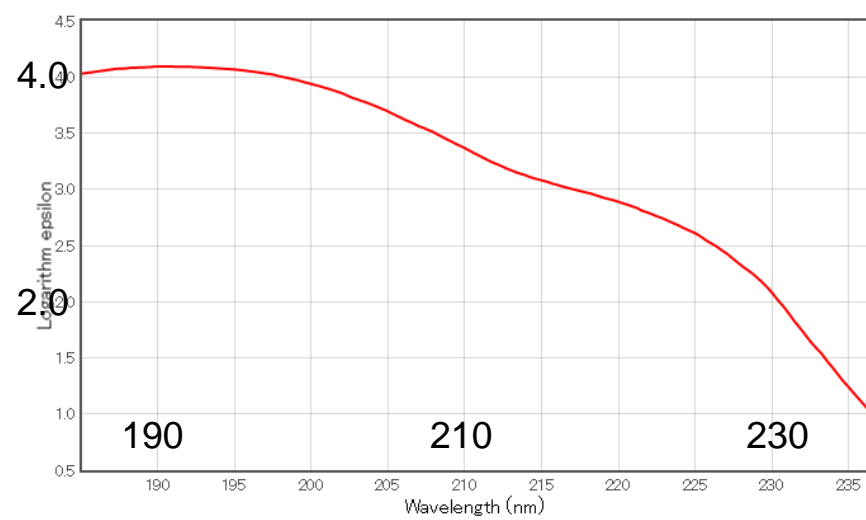


# 置換アルケンのUV/visスペクトル UV/vis spectra of substituted alkenes

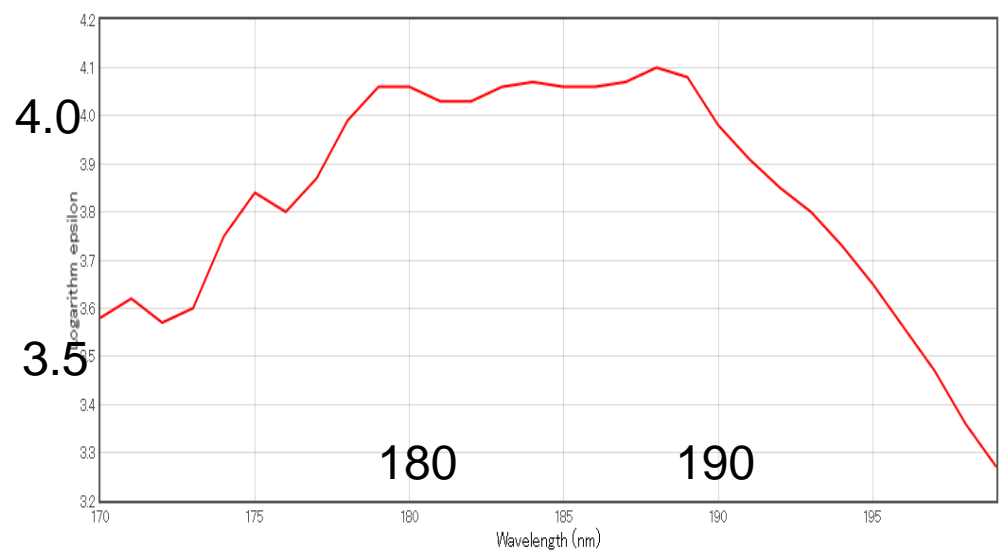
but-1-ene  $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$



2,3-dimethylbut-2-ene  $(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$



2-methylpropene  $(\text{CH}_3)_2\text{C}=\text{CH}_2$





アルキルカチオン – 空の2pz軌道への電子供与による非局在化

alkyl cations – delocalization by donation of electrons  
toward unoccupied 2pz orbital.

methane -13.01 kcal/mol

methyl cation 256.55 kcal/mol

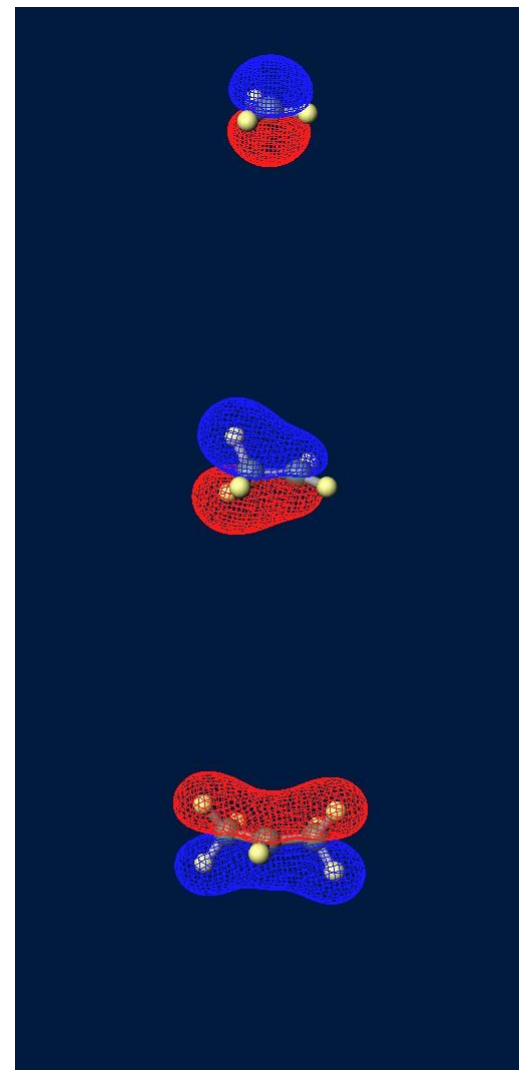
ethane -18.13 kcal/mol

ethyl cation 222.56 kcal/mol

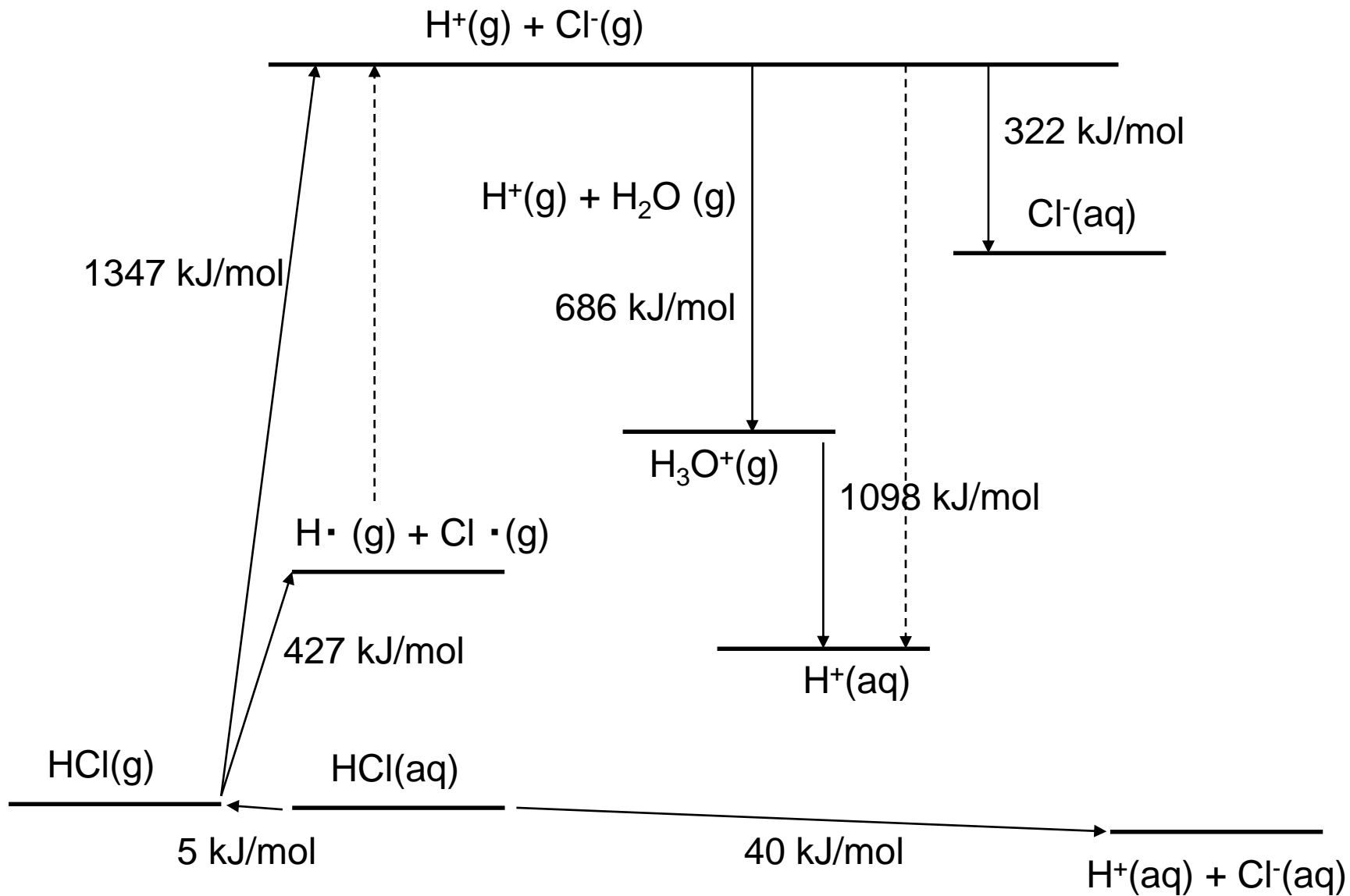
propane -23.62 kcal/mol

2-propyl cation 197.25 kcal/mol

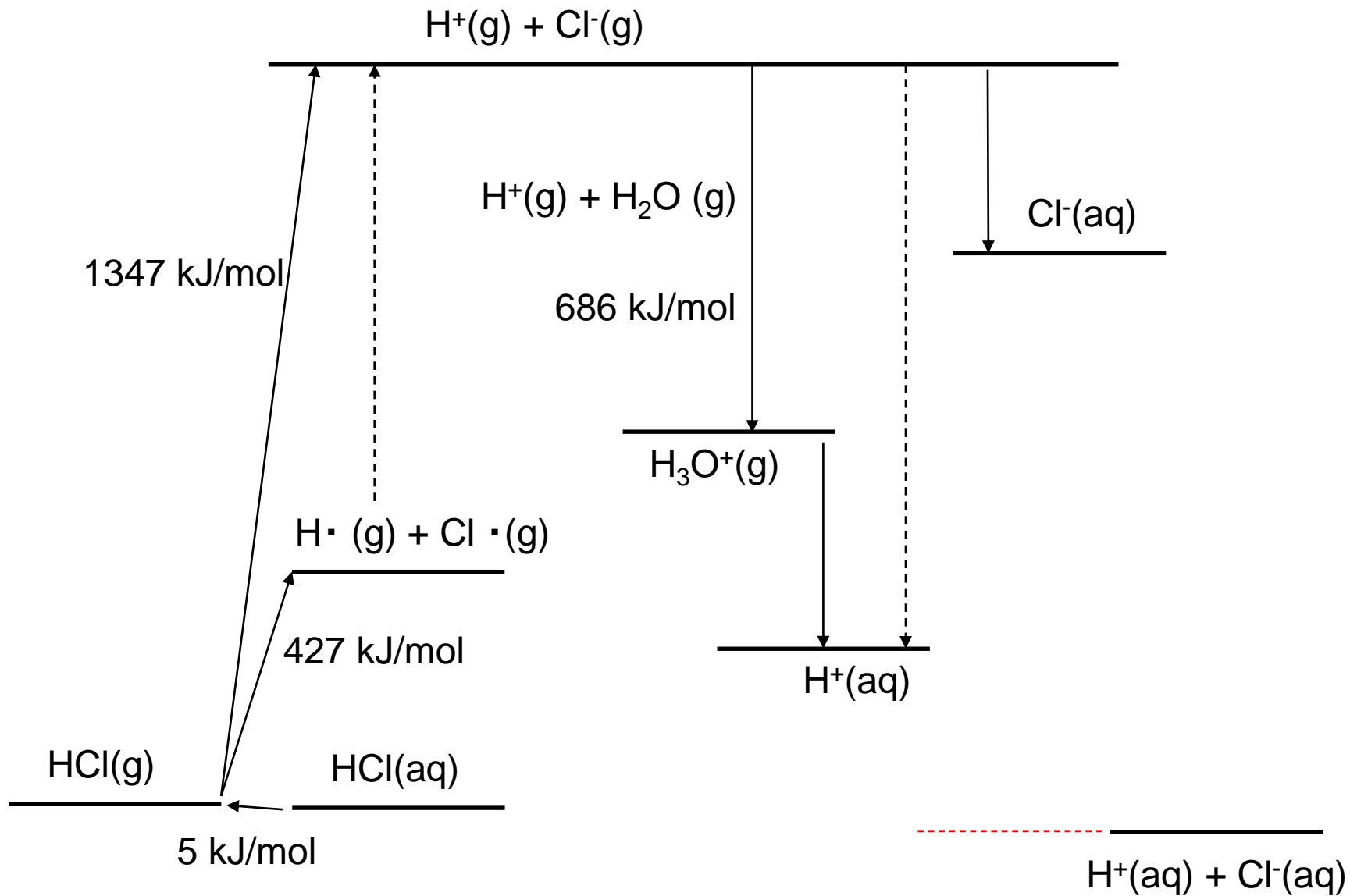
cf. 1-propyl cation 214.36 kcal/mol



# HClの解離と水和エネルギー

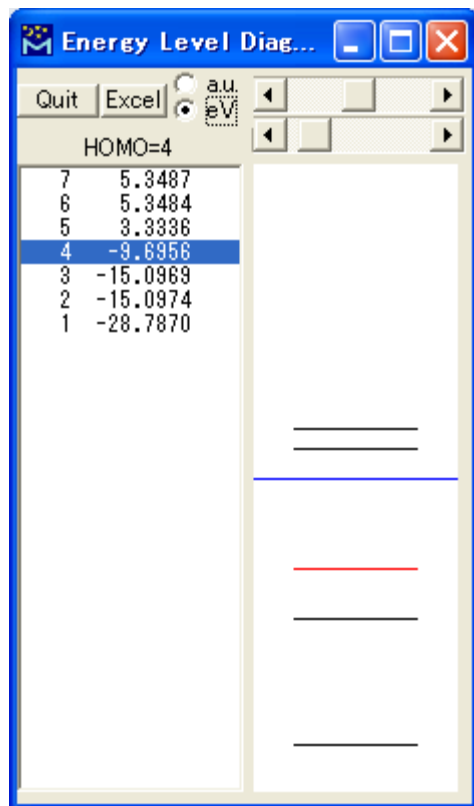


# HClの解離と水和エネルギー

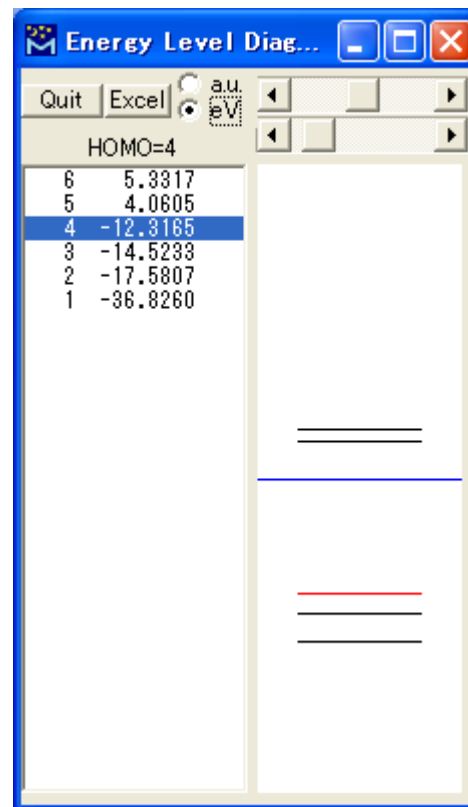


# 塩基性とHOMOのレベル

## アンモニアのHOMO

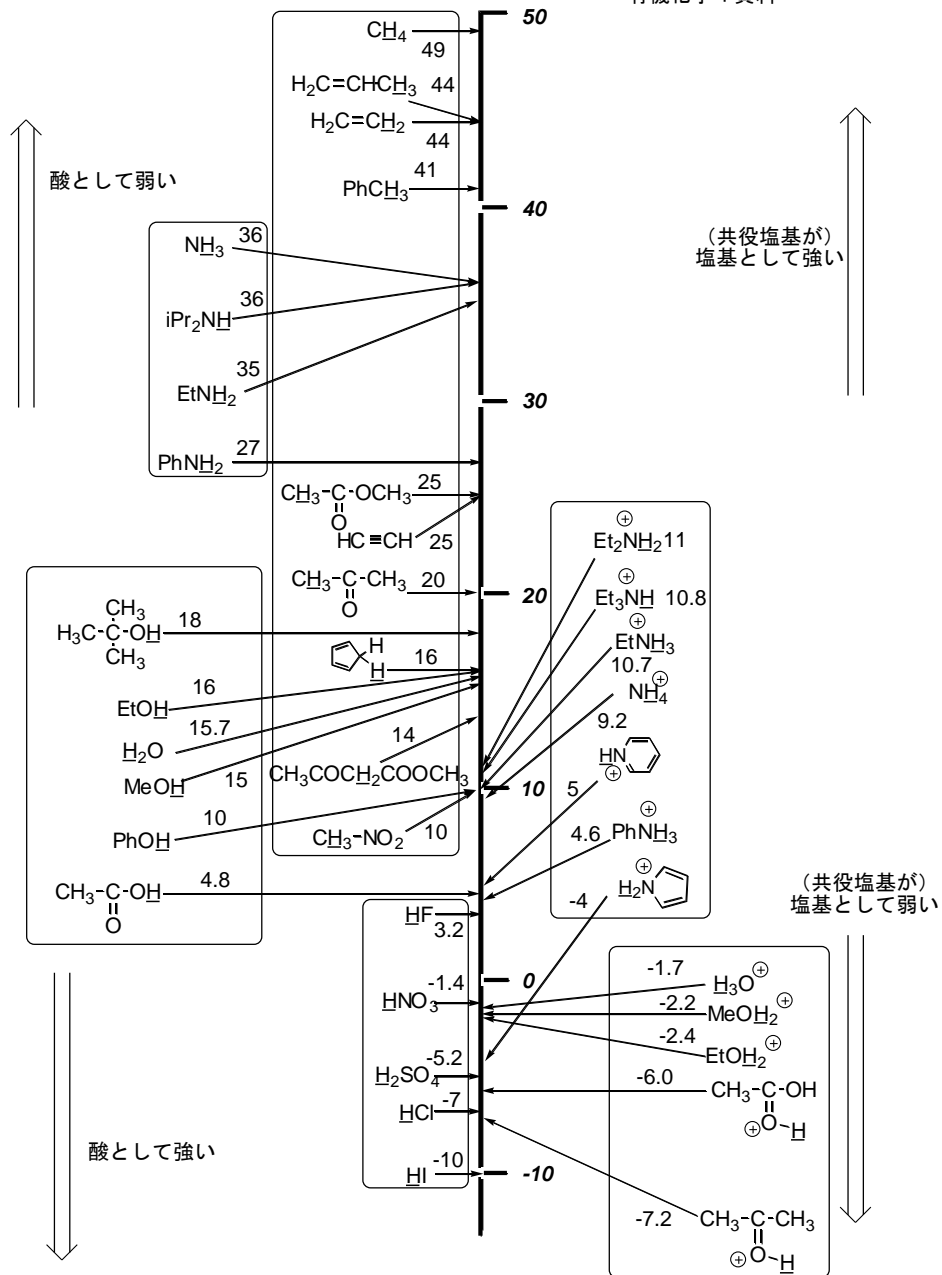


## 水のHOMO



水中での値に換算したpKa値

有機化学 1 資料



# Periodic Table of the Elements

## College of Saint Benedict / Saint John's University

With covalent radii in Angstroms ( $10^{-10}$  m); based on data from Cambridge Crystallographic Database.<sup>1</sup>

H 0.31																	He 0.28
Li 1.28	Be 0.96											B 0.84	C 0.76	N 0.71	O 0.66	F 0.57	Ne 0.58
Na 1.66	Mg 1.41											Al 1.21	Si 1.11	P 1.07	S 1.05	Cl 1.02	Ar 1.06
K 2.03	Ca 1.76	Sc 1.70	Ti 1.60	V 1.53	Cr 1.39	Mn 1.39	Fe 1.32	Co 1.26	Ni 1.24	Cu 1.32	Zn 1.22	Ga 1.22	Ge 1.20	As 1.19	Se 1.20	Br 1.20	Kr 1.16
Rb 2.20	Sr 1.95	Y 1.90	Zr 1.75	Nb 1.64	Mo 1.54	Tc 1.47	Ru 1.46	Rh 1.42	Pd 1.39	Ag 1.45	Cd 1.44	In 1.42	Sn 1.39	Sb 1.39	Te 1.38	I 1.39	Xe 1.40
Cs 2.44	Ba 2.15	Lu 1.87	Hf 1.75	Ta 1.70	W 1.62	Re 1.51	Os 1.44	Ir 1.41	Pt 1.36	Au 1.36	Hg 1.32	Tl 1.45	Pb 1.46	Bi 1.48	Po 1.48	At 1.50	Rn 1.50
Fr 2.60	Ra 2.21																
		La 2.07	Ce 2.04	Pr 2.03	Nd 2.01	Pm 1.99	Sm 1.98	Eu 1.98	Gd 1.96	Tb 1.94	Dy 1.92	Ho 1.92	Er 1.89	Tm 1.90	Yb 1.87		
		Ac 2.15	Th 2.06	Pa 2.00	U 1.96	Np 1.90	Pu 1.87	Am 1.80	Cm 1.69								

1. Beatriz Cordero et al. *Dalton Trans.* **2008**, 21,;2832–2838.

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