有機化学研究におけるNMR

Allyl cation

Journal of the American Chemical Society, vol. 86, pp.5682-83 (1964)

Stable Carbonium Ions. XII.[1] Direct Observation of the Allyl and 2-Methylallyl Cations

TABLE I

N.M.R. SHIFTS OF THE ALLYL AND METHYLALLYL CATIONS AS HEXAFLUOROANTIMONATE COMPLEXES IN SO_2–SbF_5 SOLUTION AT −60°[a]

	$=CH_2$		$-CH-$	$-CH_2F$	$-CH_3$
$CH_2{=}CH{-}CH_2{-}F$ (in SO_2)	−5.14 (*trans*)	−5.01 (*cis*)	−5.52	−4.56 (J_{HF} = 47.5)	
$[CH_2{=}CH{=}CH_2]^+SbF_6^-$	−8.97		−9.64		
$CH_2{=}C(CH_3){-}CH_2{-}F$ (in SO_2)	−4.81	−4.69		−4.32 (J_{HF} = 46)	−1.47
$[CH_2{=}C(CH_3){=}CH_2]^+SbF_6^-$		−8.95			−3.85

[a] P.p.m. from external $(CH_3)_4Si$.

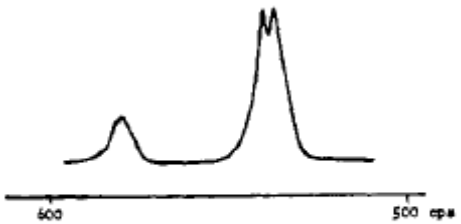

Fig. 1.—Proton magnetic reasonance spectrum of the allyl cation in SbF_5–SO_2 at −60° (60 Mc., external TMS).

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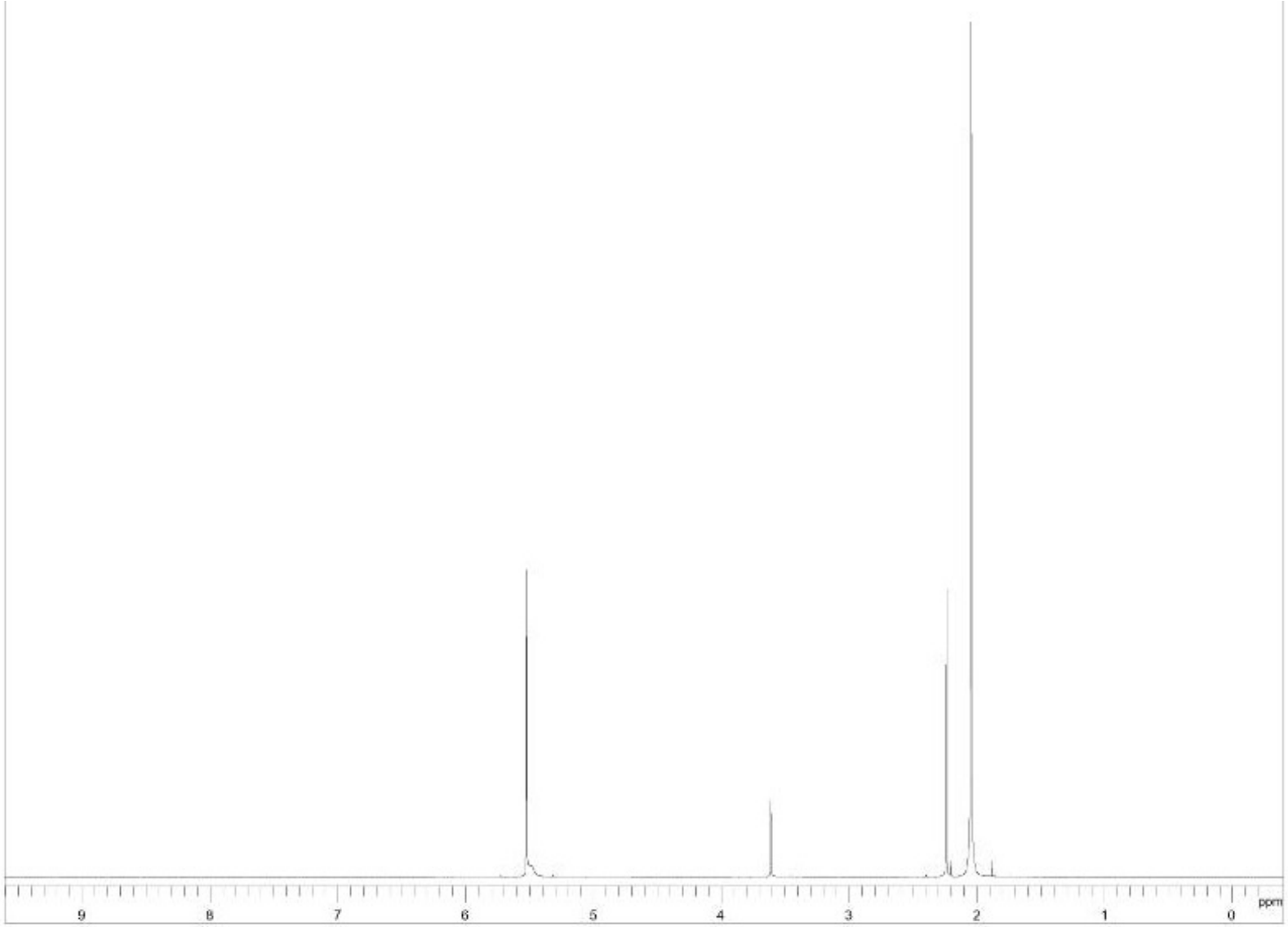
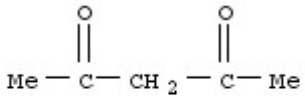
ケトーエノール互変異性



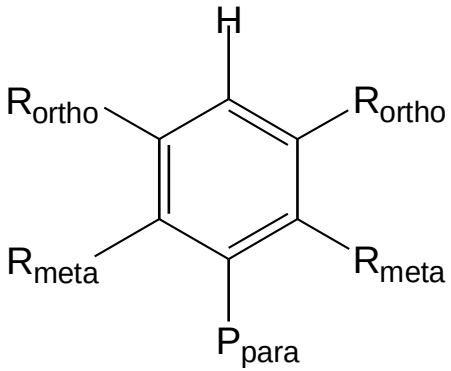
CAS Registry Number: 123-54-6

$C_5H_8O_2$

2,4-Pentanedione



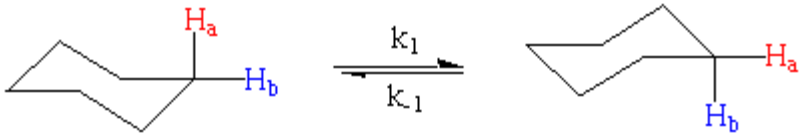
ベンゼン環プロトンの化学シフトへの置換基効果



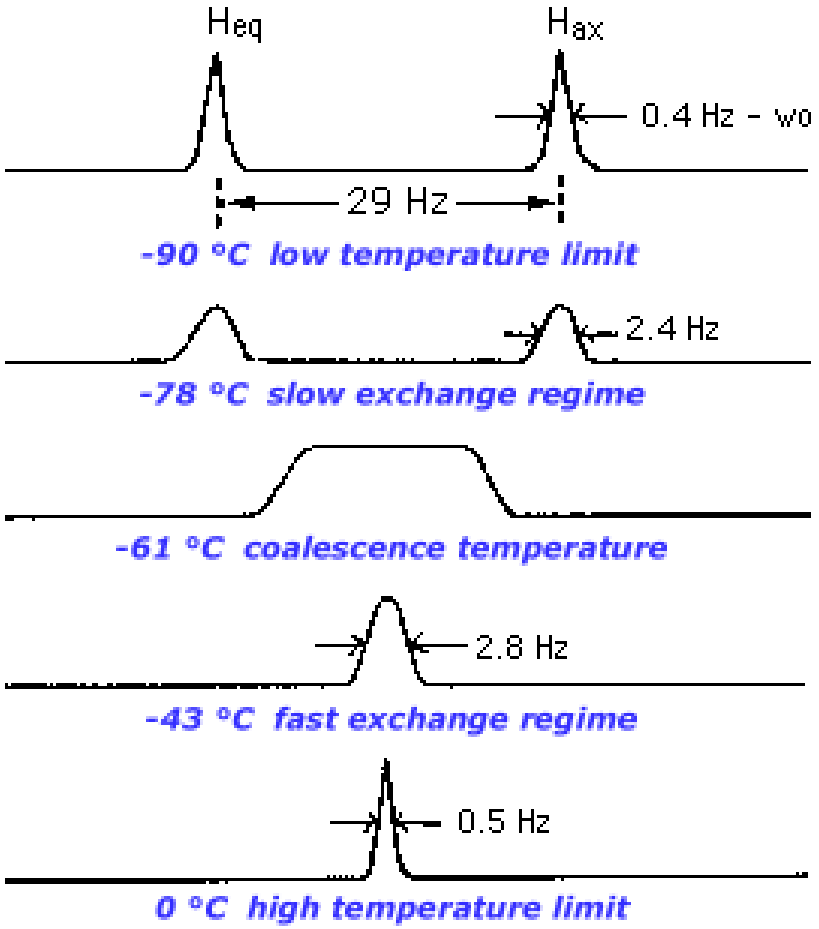
Base : 7.27

置換基 (R)	ortho	meta	para
–NMe_2	-0.60	-0.10	-0.62
–NH_2	-0.75	-0.24	-0.63
–OH	-0.50	-0.14	-0.40
–Me	-0.17	-0.09	-0.18
–Cl	0.02	-0.06	-0.04
–Br	0.22	-0.13	-0.03
–Ph	0.18	0	-0.08
–CN	0.27	0.11	0.30
–CO_2H	0.80	0.14	0.20
–NO_2	0.95	0.17	0.33

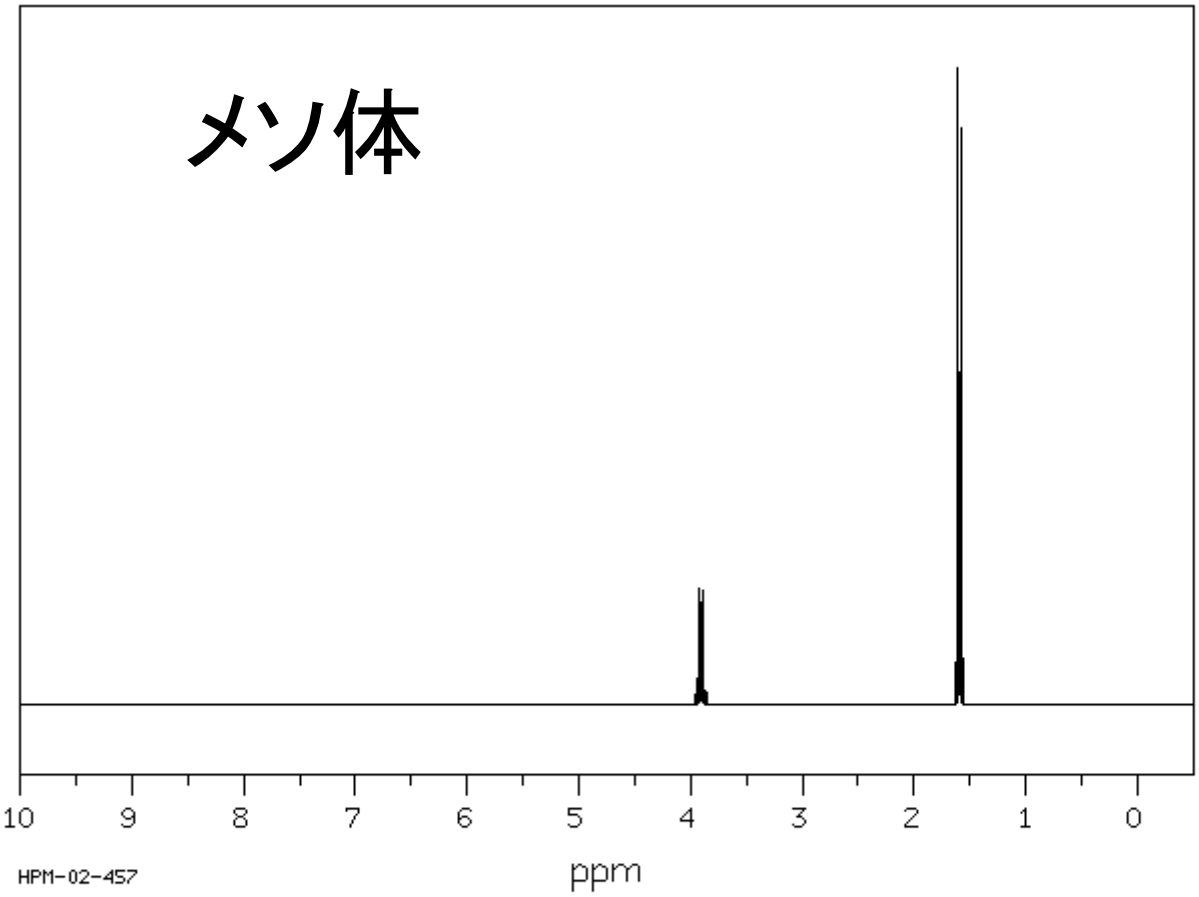
シクロヘキサンの運動性

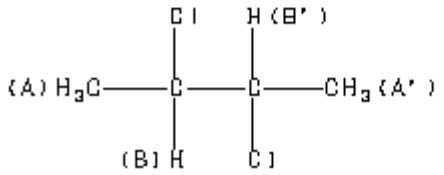


coalescence： 合体，癒着



ジアステレオマー(1)





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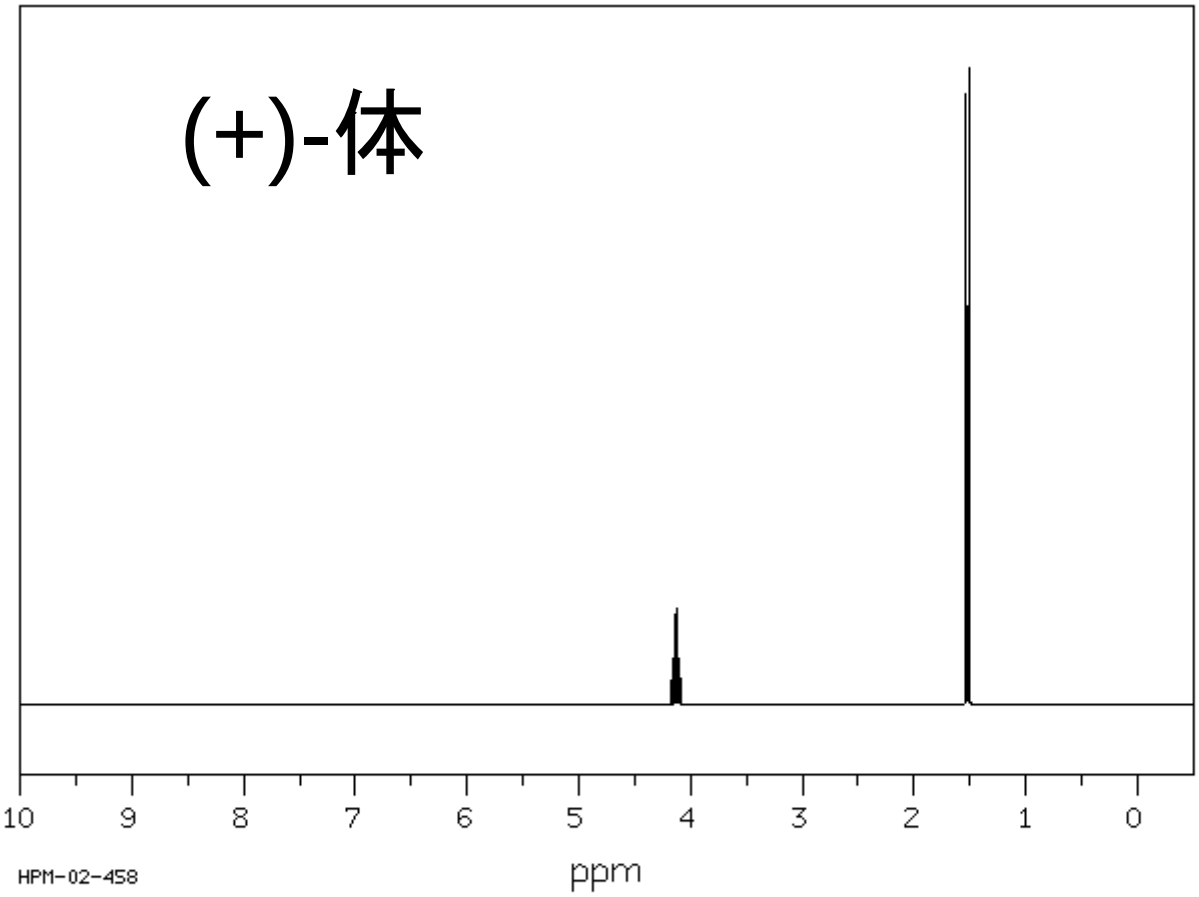

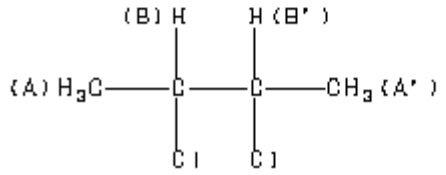

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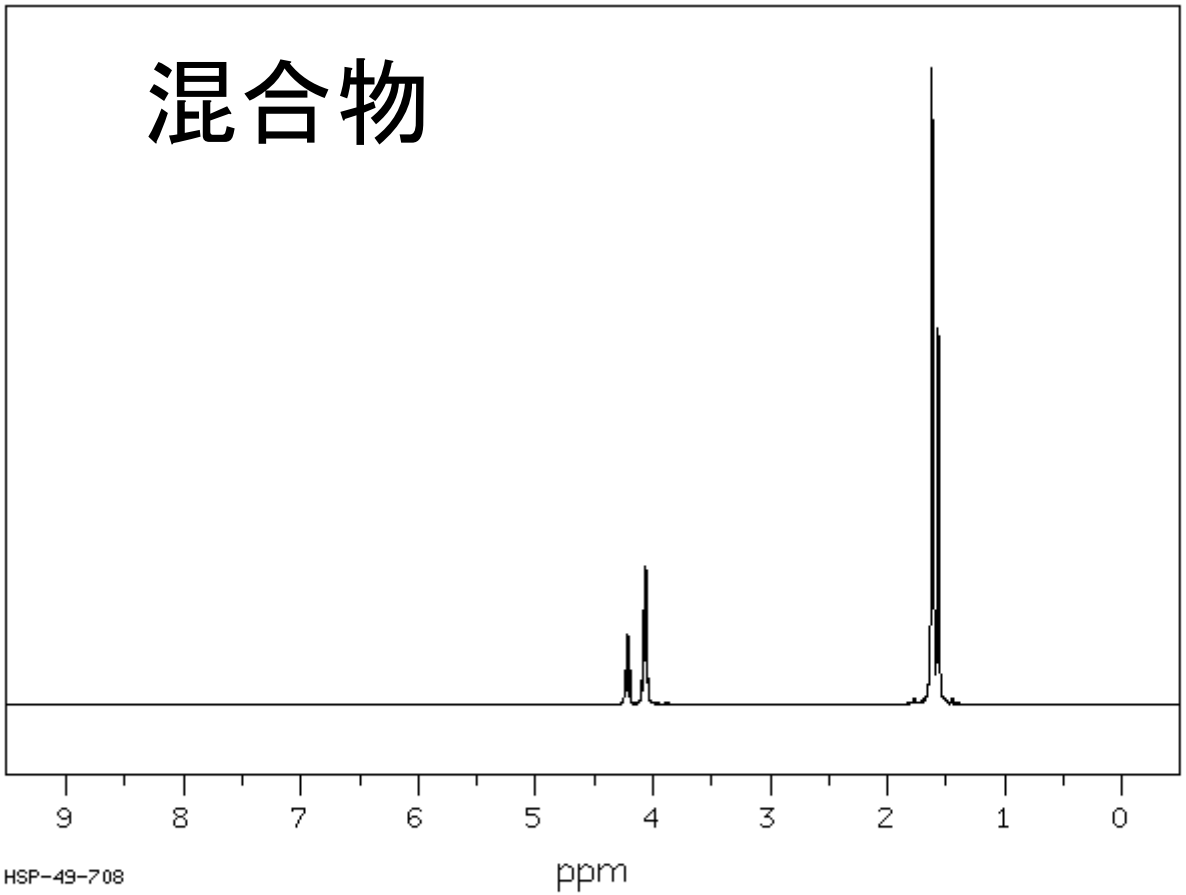

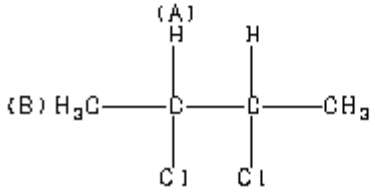

実験科学の基本的流れ（１）

１．実験

　１－１．作業仮説の提唱
　１－２．仮説の検証（実験）
　１－３．仮説の修正
　１－４．（１－２へもどる）

２．結果の解釈と理論の構築―帰納―
［自身の実験結果と既知の理論・他人の実験結果との整合性が必要］

３．理論の正当性の確認―演繹―

実験科学の基本的流れ（２）

・子曰、学而不思則罔、思而不学則殆。

・理論どおりのことが起こらなかったときが発見の第一歩