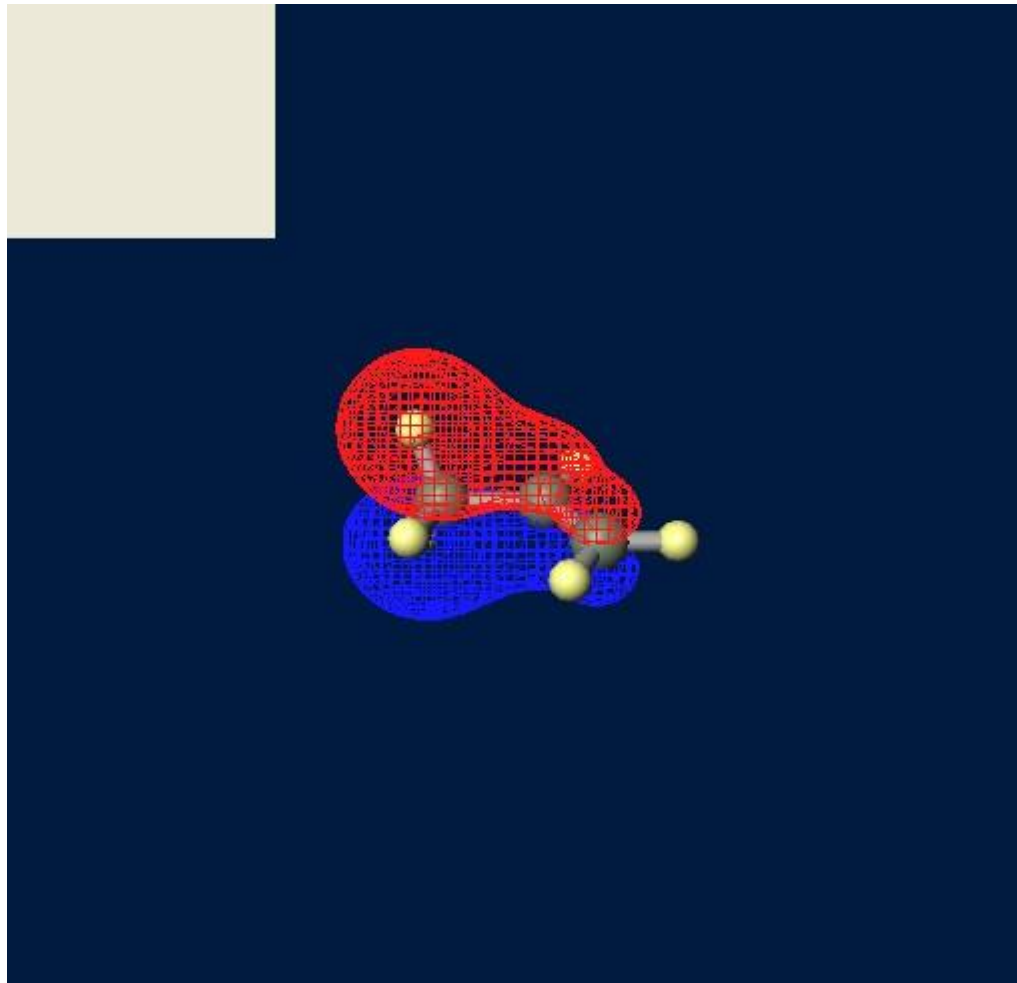


propeneの π 性の分子軌道2 (被占軌道)



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 $\text{SO}_2\text{-SbF}_5$ SOLUTION AT -60°a

	=CH_2		—CH—	$\text{—CH}_2\text{F}$	—CH_3
$\text{CH}_2=\text{CH—CH}_2\text{—F}$ (in SO_2)	-5.14 (<i>trans</i>)	-5.01 (<i>cis</i>)	-5.52	-4.56 ($J_{\text{HF}} = 47.5$)	
$[\text{CH}_2=\text{CH—CH}_2]^+\text{SbF}_6^-$		-8.97	-9.64		
$\text{CH}_2=\text{C}(\text{CH}_3)\text{—CH}_2\text{—F}$ (in SO_2)	-4.81	-4.69		-4.32 ($J_{\text{HF}} = 46$)	-1.47
$[\text{CH}_2=\text{C}(\text{CH}_3)\text{—CH}_2]^+\text{SbF}_6^-$		-8.95			-3.85

^a P.p.m. from external $(\text{CH}_3)_4\text{Si}$.

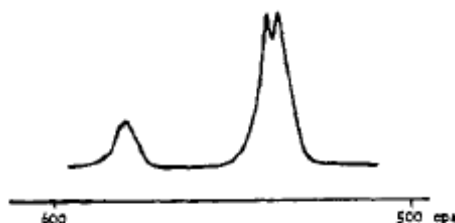


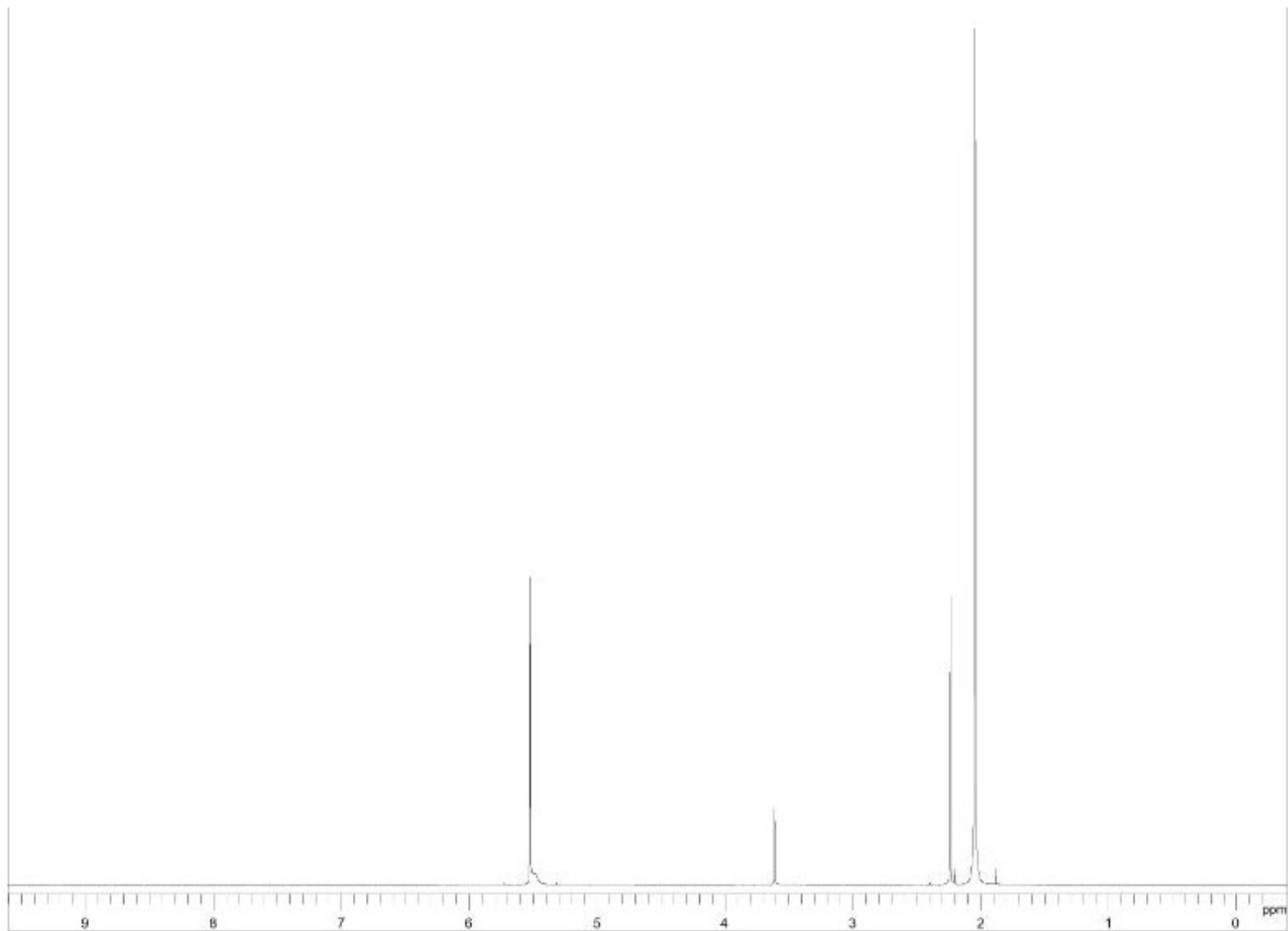
Fig. 1.—Proton magnetic resonance spectrum of the allyl cation in $\text{SbF}_5\text{-SO}_2$ at -60° (60 Mc., external TMS).

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GEORGE A. OLAH
MELVIN B. COMISAROW

RECEIVED SEPTEMBER 23, 1964

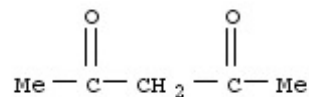
ケト-エノール互変異性



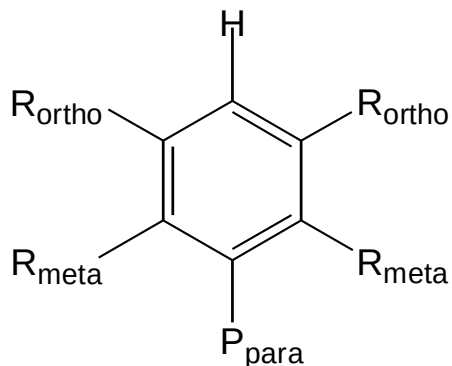
CAS Registry Number: 123-54-6

C₅ H₈ O₂

2,4-Pentanedione



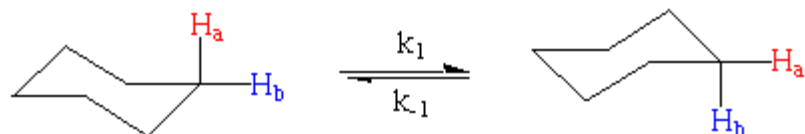
ベンゼン環プロトンの化学シフトへの置換基効果



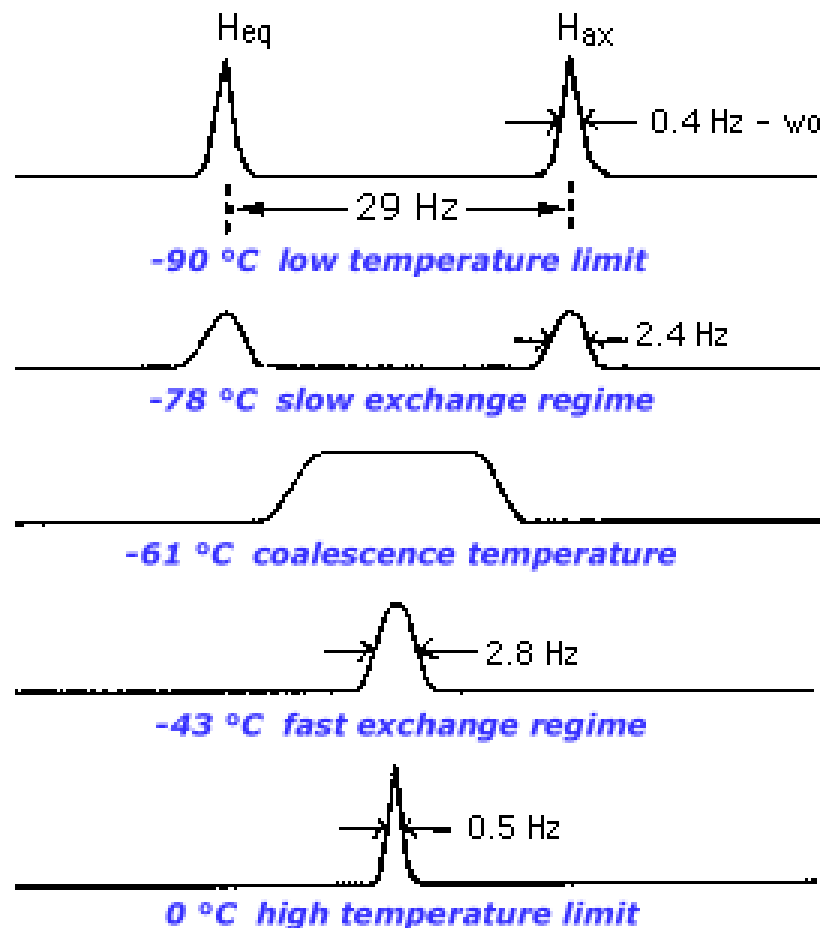
Base : 7.27

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 ₂ H	0.80	0.14	0.20
-NO ₂	0.95	0.17	0.33

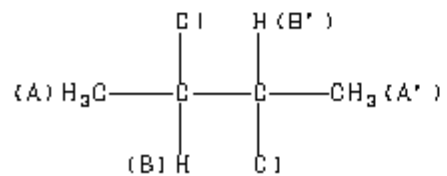
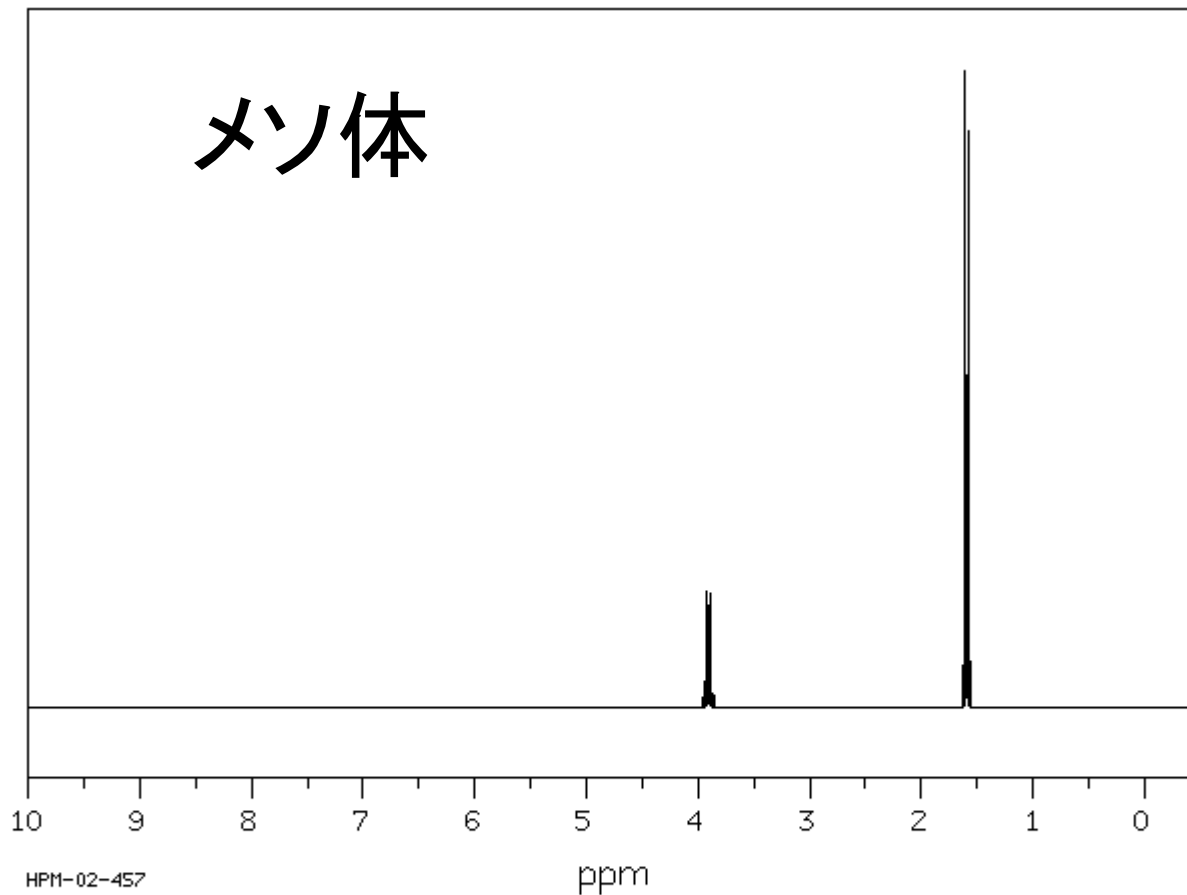
シクロヘキサンの運動性



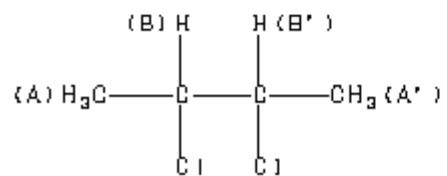
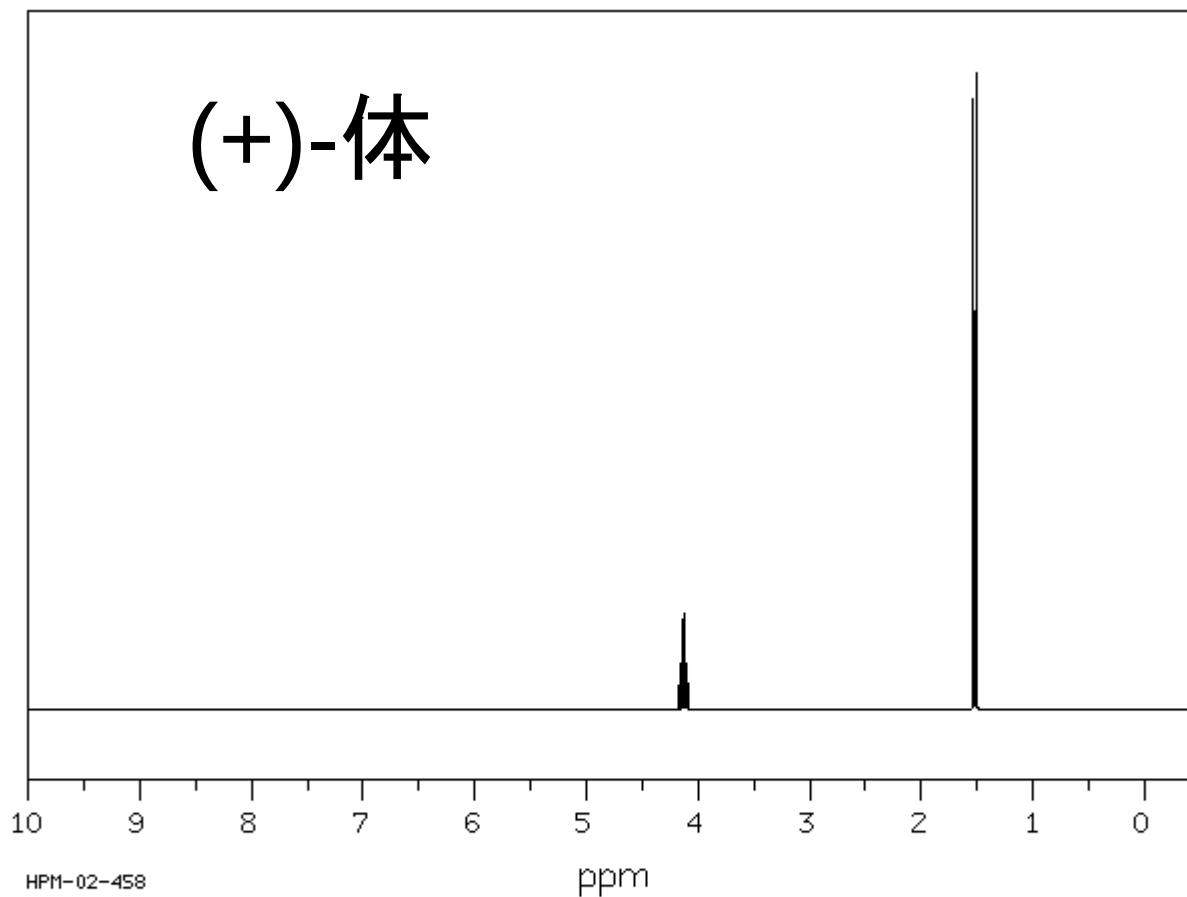
coalescence : 合体, 癒着



ジアステレオマー(1)

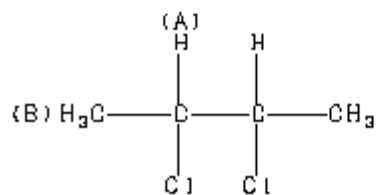
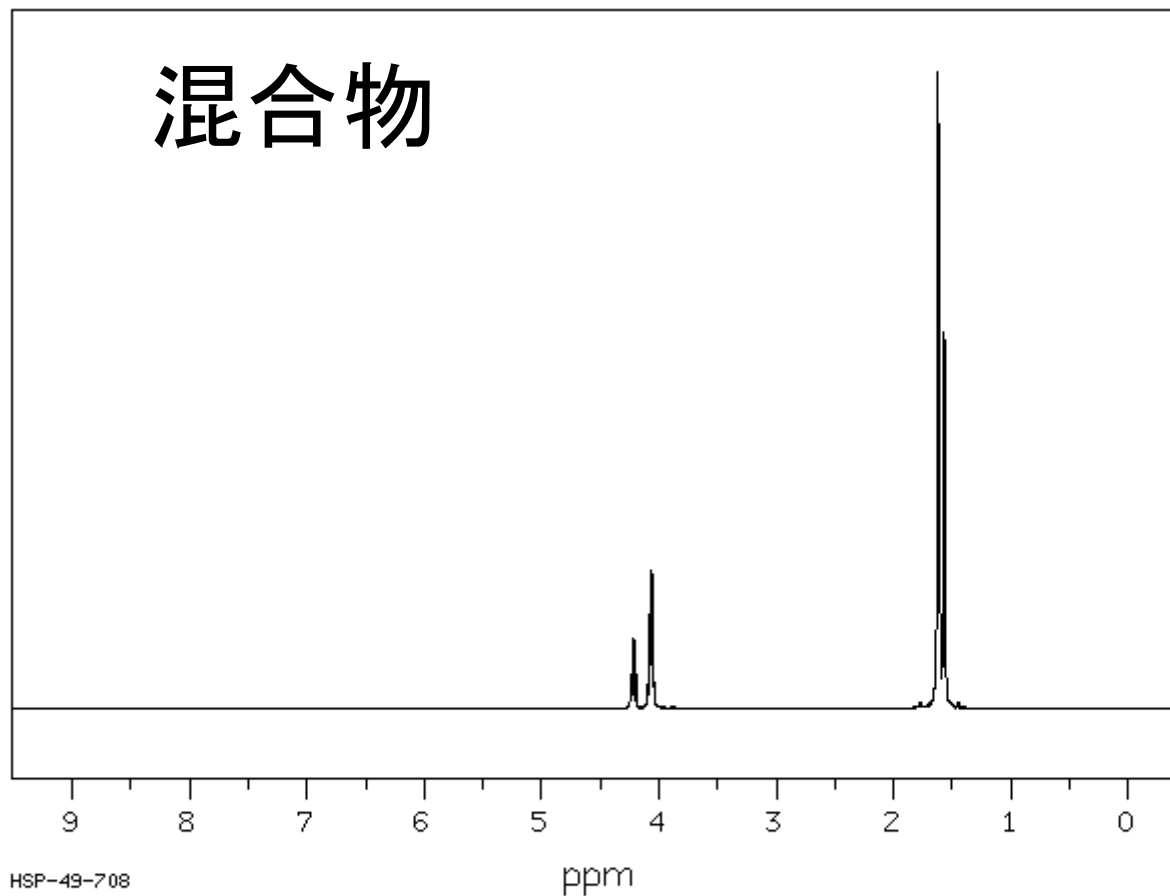


ジアステレオマー(2)



ジアステレオマー(3)

混合物





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