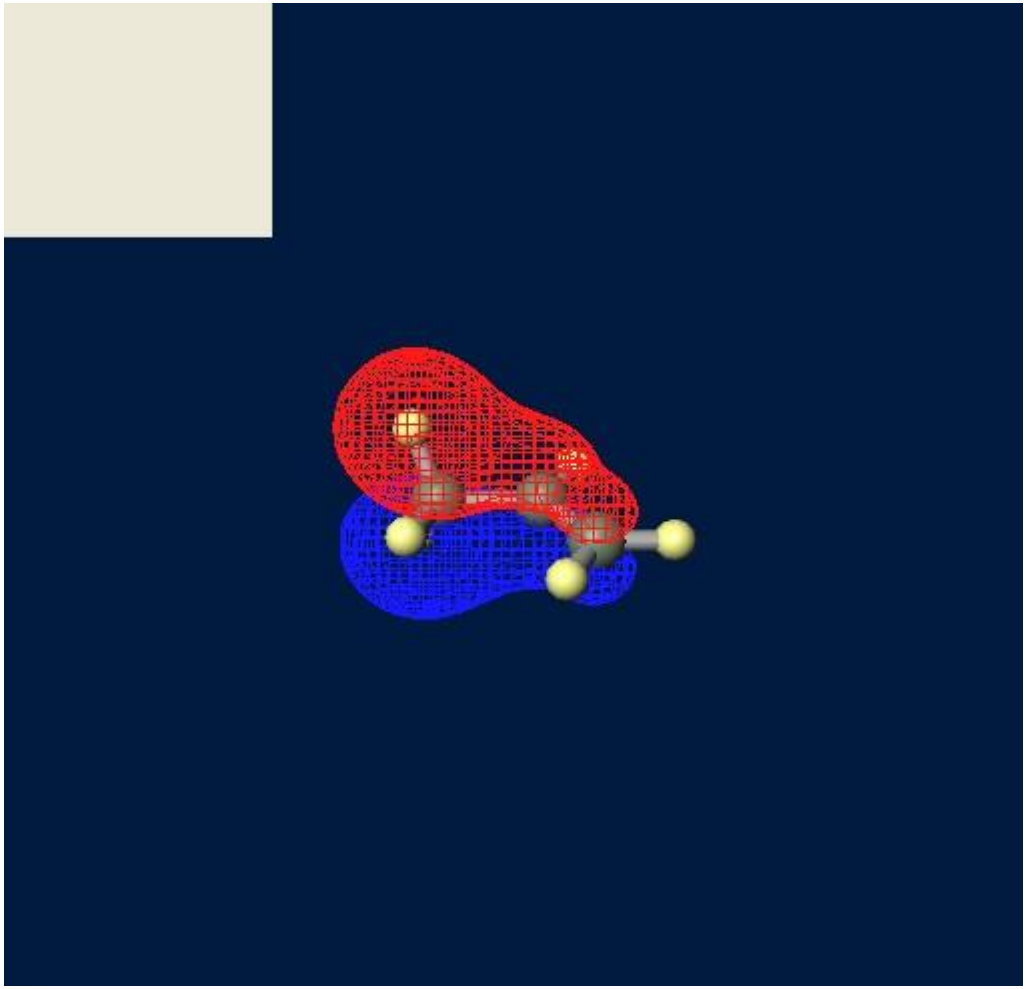
propeneのπ性の分子軌道2（被占軌道)



# 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 $SO_2$–$SbF_5$ 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 $(CH_3)_4Si$.

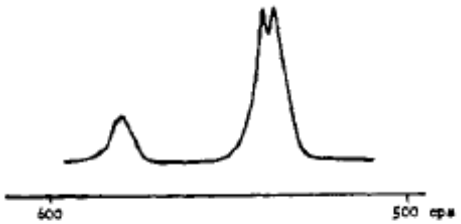



Fig. 1.—Proton magnetic reasonance spectrum of the allyl cation in $SbF_5$–$SO_2$ at −60° (60 Mc., external TMS).

THE DOW CHEMICAL COMPANY
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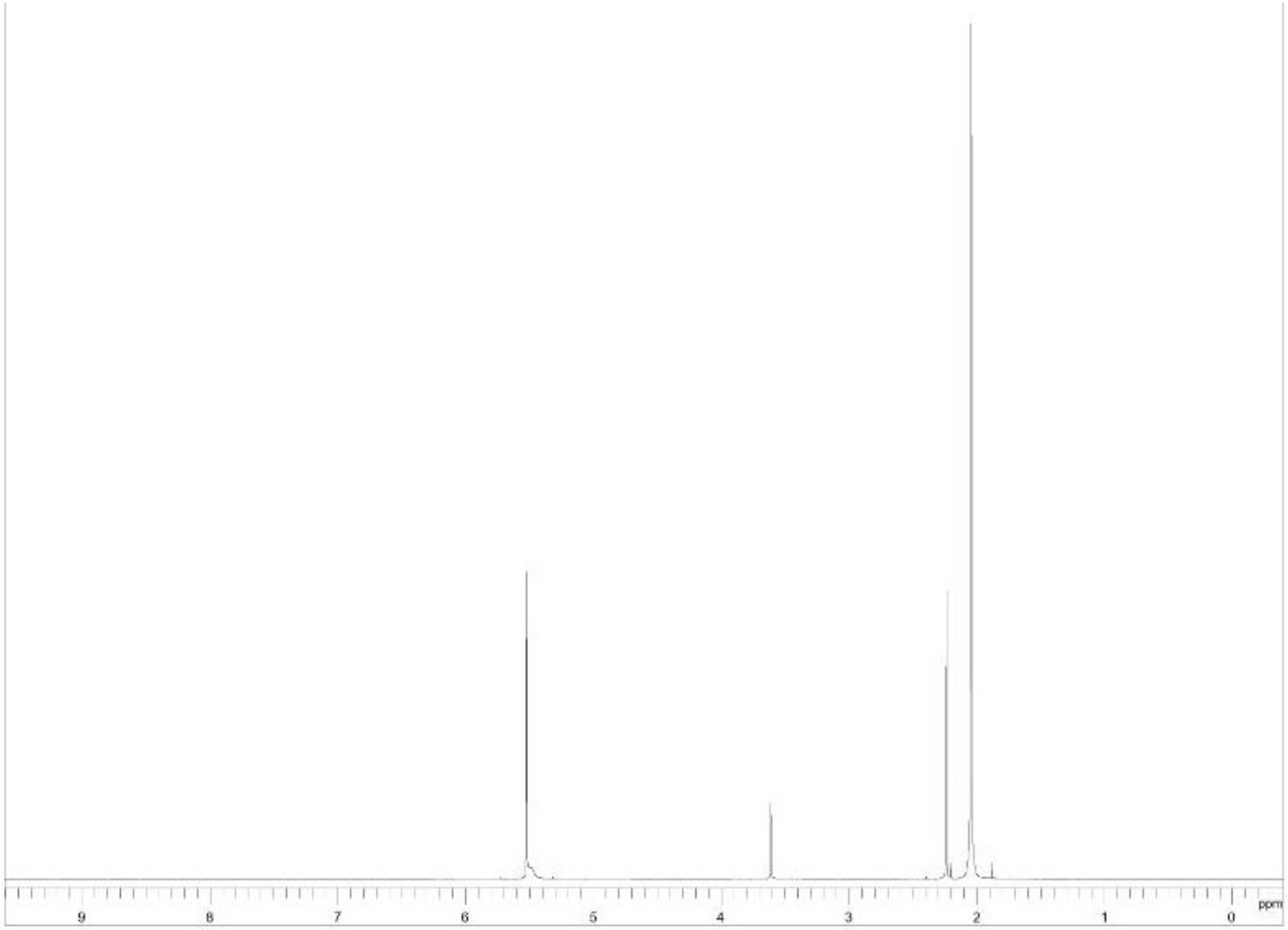
GEORGE A. OLAH
MELVIN B. COMISAROW

RECEIVED SEPTEMBER 23, 1964

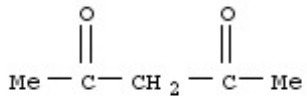
# ケトーエノール互変異性



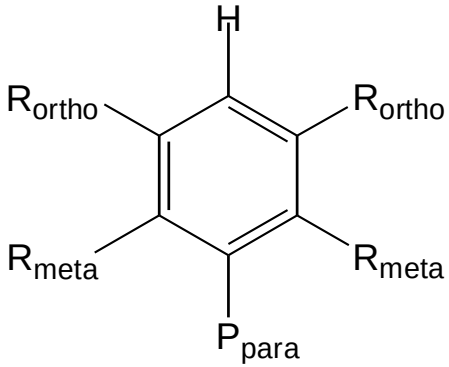

**CAS Registry Number:** 123-54-6

$C_5H_8O_2$

2,4-Pentanedione



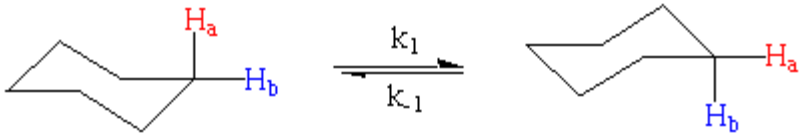
# ベンゼン環プロトンの化学シフトへの置換基効果



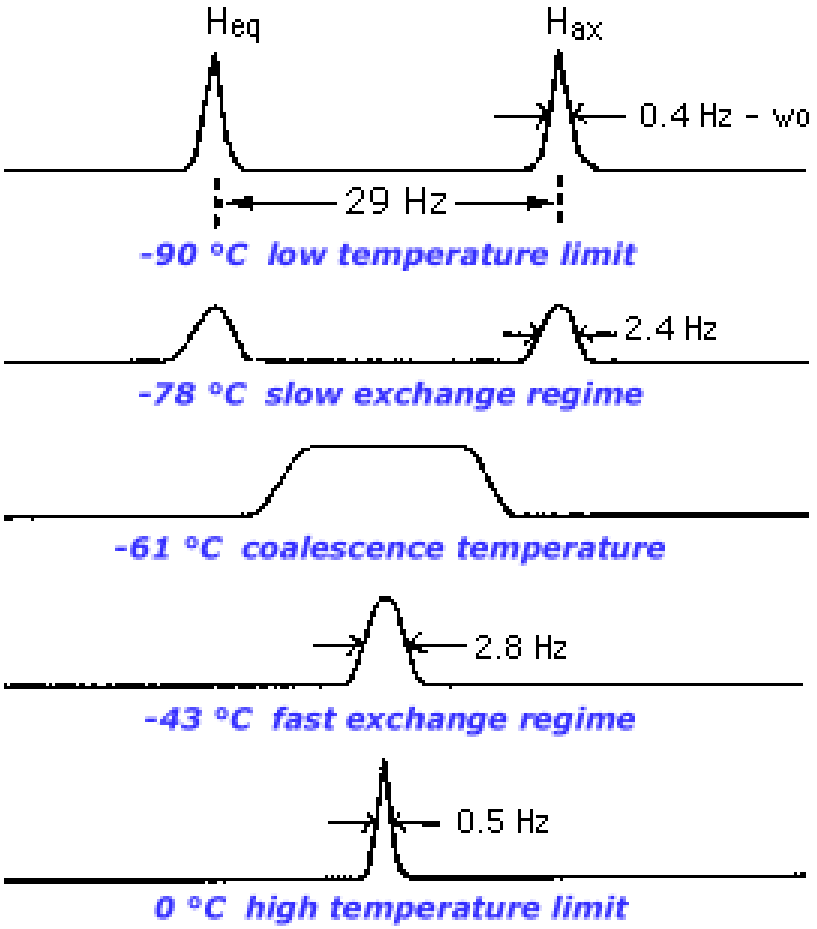

Base : 7.27

| 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 |

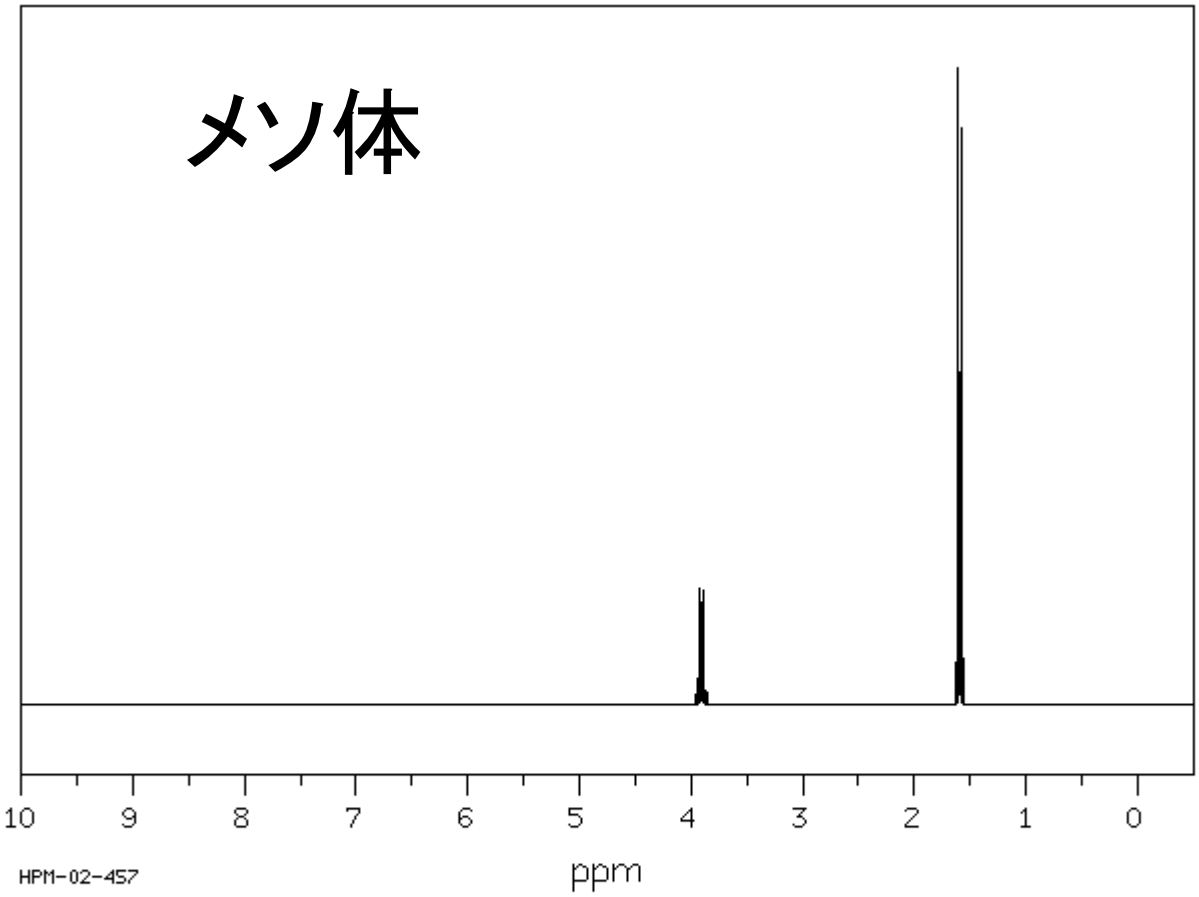
# シクロヘキサンの運動性

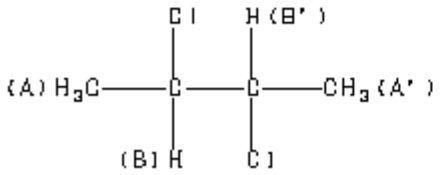



coalescence： 合体，癒着



# ジアステレオマー(1)



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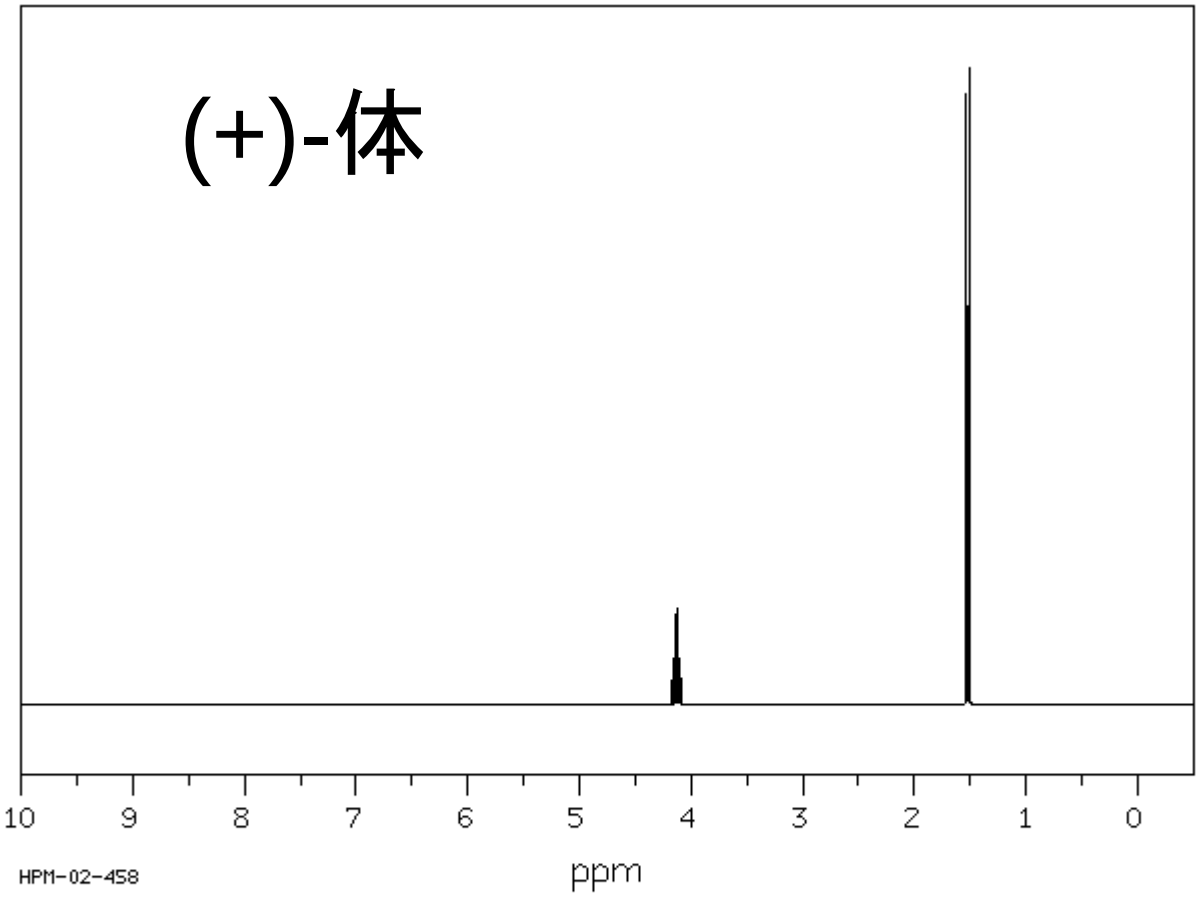


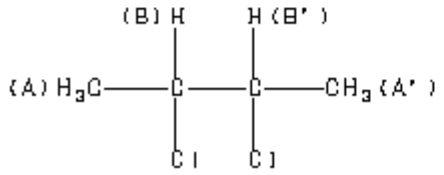

# ジアステレオマー(3)