

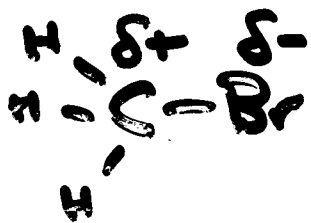
# NUCLEOPHILIC SUBSTITUTION.

CONSIDER THE FOLLOWING:



SUBSTITUTION RXN I FOR Br  
ON ORGANIC UNIT.

$\text{I}^{\ominus}$  (IODIDE ION) - NUCLEOPHILE  
(BRINGS ELECTRON PAIR INTO  
RXN)



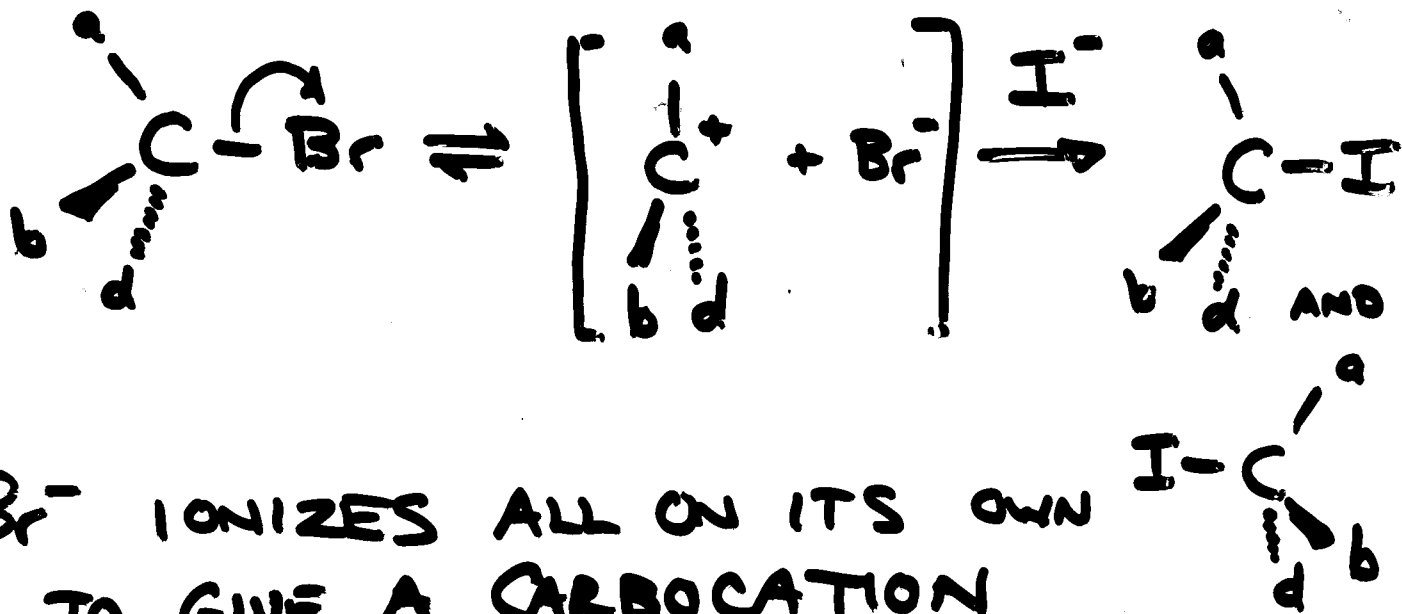
CONSIDERED THE  
ELECTROPHILE, BY  
VIRTUE OF ELECTRONEGATIVITY  
OF Br

- SOMETHING MUST LEAVE WITH AN  $e^-$  PAIR.  $\text{Br}^{\ominus}$  IS ONLY CHOICE
- $\text{Br}^{\ominus}$  IS THE 'LEAVING GROUP'
- $\therefore$  CALLED NUCLEOPHILIC SUBSTITUTION

# TWO LIMITING MECHANISMS.

## $S_N1$ Rxn. - THE CARBOCATION ROUTE.

- POSSIBLE TO.....



- Br<sup>-</sup> IONIZES ALL ON ITS OWN TO GIVE A CARBOCATION

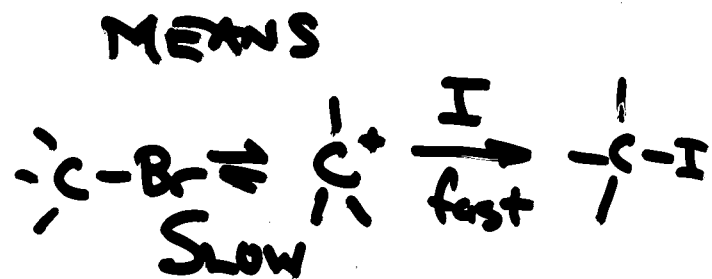
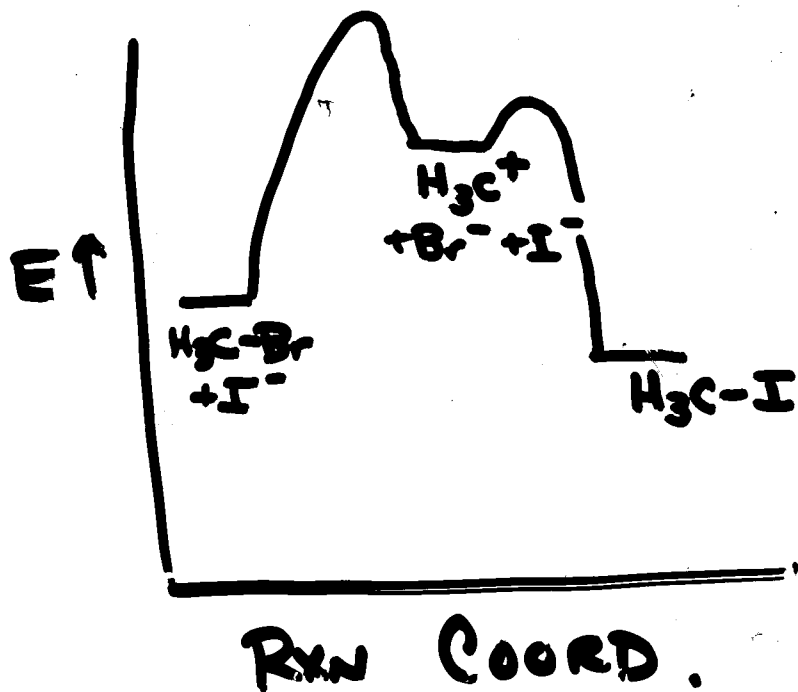
- CARBOCATION THEN COMBINES WITH THE NUCLEOPHILIC I<sup>-</sup> ION.

- THERE IS AN INTERMEDIATE

- RYN ENERGETICS PROFILE

- TOUGH THING IS TO SEPARATE A NEUTRAL MOLECULE INTO 2 IONS.

∴ 1<sup>ST</sup> STEP IS TOUGHEST/SLOWEST



RATE  $v = k [\text{CH}_3\text{-Br}]$   
 OR  $k [\text{R-X}]$

$\therefore$  1<sup>ST</sup> ORDER RXN

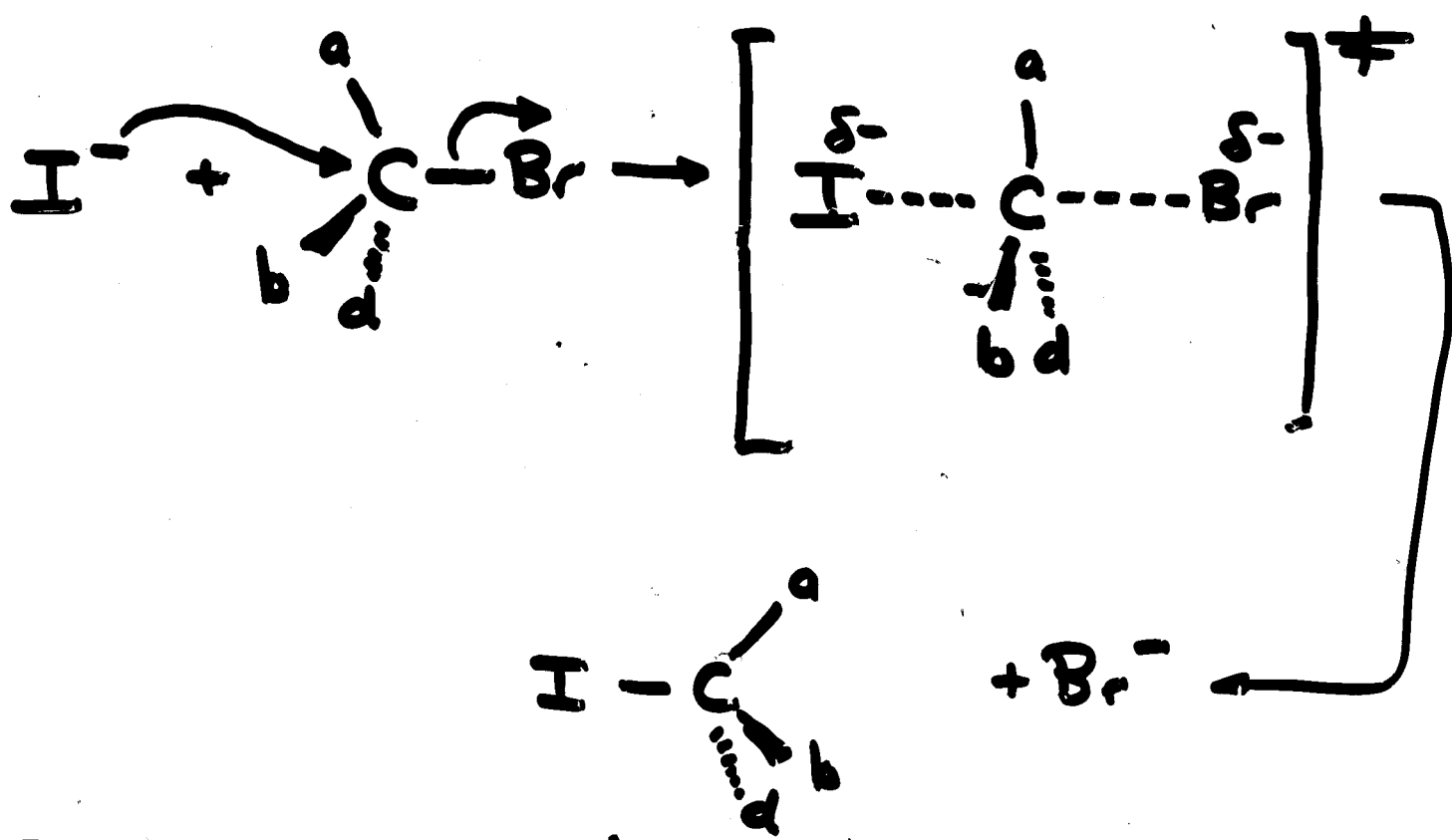
$\therefore$  S<sub>N</sub>1 RXN.

ALTERNATIVE # 2

S<sub>N</sub>2 RXN. - CONCERTED ROUTE

- CASE WHERE THE STEPS ARE ALL HAPPENING AT THE SAME

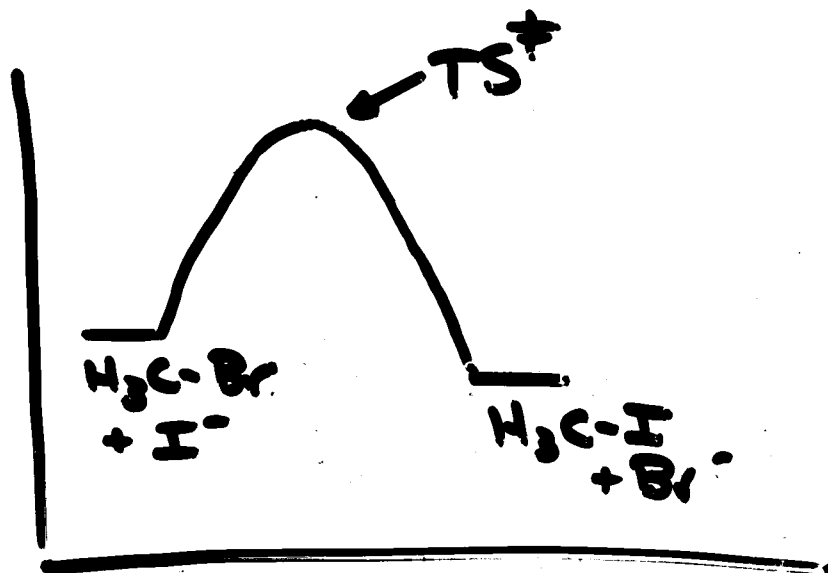
- C-Br BOND BREAKING, I-C BOND IS FORMING, I IS LOSING ITS CHARGE, Br IS GAINING ITS CHARGE



REALLY ONLY 1 STEP

- NO INTERMEDIATE ; INSTEAD THERE IS A TRANSITION STATE.

- ENERGETICS



RATE  $\propto k [CH_3-Br] [I^-]$   
 OR  $k [R-X] [Nu]$

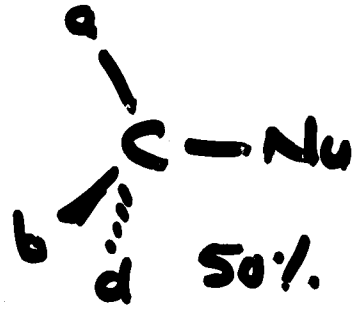
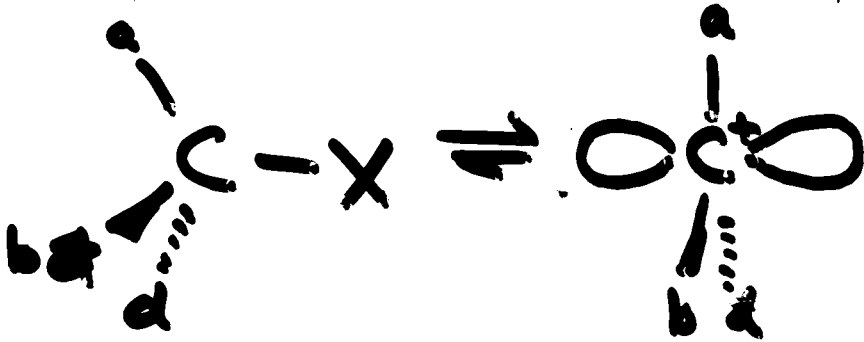
2<sup>ND</sup> ORDER

$S_N2$  MECHANISM

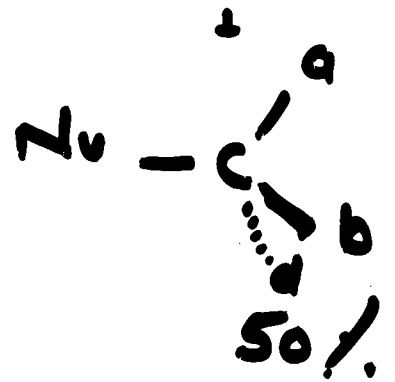
STEREOCHEMISTRY OF RXN.

- BIG DIFFERENCE BETWEEN  $S_N1$  AND  $S_N2$ .

$S_N1$



NO PREFERENCE FOR  $Nu^-$  TO COME IN FROM SIDE VS THE OTHER



$\therefore$  GET RACEMIC MIXTURE

- IF START WITH ONE CHIRAL CENTRE, GET RACEMIZATION AT THAT CENTRE

- IF YOU HAVE 2. CHIRAL CENTRES + 1 REACTING, GET DIASTEREOMERS.

