(2)The Br2  form a bridgehead

# TOP SIDE ANTI ATTACK

(1) Initial approach of Br2  in a topside, anti attack across trans—cinnamic acid

because the pi e- initiates attack forces a cascade of e- motion shown below leading to Br-Br bond breakage. The alkene moiety lengthens as the pi system dissolves. The COOH side is favored for reasons discussed in (3)



(3)

(3) Br-Br bond ruptures and the bridgehead dissolves. The Br across the double bond selects the COOH side since this produces a carbocation on the phenyl side, which is stabilizing because of the deolcalization of the aromatic electron. The COOH side flexes downwards away from the Br now sharing its C attachment so that the bonding on that side moves from sp2🡪 sp3 .The remaining Br becomes a bromide ion (Br -) and the carbocation site is sp2 , e.g. it goes flat.



(4) The remaining Br- now attacks from the back (anti side) to neutralize the carbocation. The phen and H flex upwards, and the sp2 hybridization converts to sp3







(4)

**a**

(5)



(5) rotation of the final product in step (4) to make the rotational isomer with phen and COOH eclipsing each other leads to the final erythro form (3S,2R) Fischer structure. This should melt at ~200oC.

**b**

**TOP SIDE SYN ATTACK**

(1)

(1) syn attack starts with both Br simultaneously donating a single e on the same side of the pi system which evenly divides its pi system in 1 e- transfers. As the Br-C bonds form, the Br-Br bond weakens and the four groups flex down in the same direction.

(3) The final structure in (2) is rotated so that the COOH and phen eclipse each other. This produces the Fischer configuration which is a threo (2R,3R) structure which melts around 95 oC



(3)

(2) Br-Br bond is now entirely broken and the new C-Br bonds have formed. The pi bond is gone and the bond length and the bon length between C2 and C3 is longer. The four groups (H,COOH) and (H,phen) are now in sp3 hybridized form.

(2)





**a**

**bv**

Some style notes:

* Make sure to use a combination of pictures and text with latter being physically close to the former on page; so that a reader can easily see what is being said in words in the accompanying picture. Use the electron pushing `curved’ arrow format wherever possible.
* Make sure critical terms and positions in pictures are well-labeled (as above)
* Use full sentences and be brief. Let the pictures do some of the work
* **GRADING RUBRIC FOR ADDITION OF Br2 ACROSS TRANS-CINNAMIC ACID** (formal Theory + Lab notebook due 7 February. total points possible: **75)**

**Lab book (25 points total)**

Purpose 3

Procedure 10

Results 7 (yield …enough for mp ; sensible mp; correct color)

Materials table 5

**Formal Theory Report (50 pts total)**

(0) Intro/Purpose (write out overall reaction; explain point of experiment) 2

(1)***Theory***

Most likely possible anti attack cases considered thoroughly\* 18

Argument for why other two anti attack cases less likely 5

both syn cases considered thoroughly 10

(2)***Table of stereo outcomes***

R,S assignments for four results listed 10

workmanship (clear language, clear diagrams, easy 5

to read and understand. English) 50

***(1)Notes on what to put in Theory***

A guide for key points in the mechanistic description of one of the four possible stereoselective anti pathways is attached. A guide for the key points for one of the two possible syn pathways is also illustrated. It is suggested that you thoroughly discuss the the two most likely anti attacks … but summarize the Fischer structures for all four possibilities of the anti mechanism. It is important that you rationalize why the pathways you discuss in detail are most likely . (hint: `phen’ group is electron rich group)

***Make sure to explain how melting pt determination allows us to decide whether anti or syn attack by Br2 occurs.***

***The four possible anti attacks (T= top, B= bottom)***

T1)top side attack, Br attaches first to COOH side, then backside attack on phen end

T2)top side attack, Br attaches first to phen side, then backside attack on COOH end

B1)bottom side attack, Br attaches first to COOH side, then backside attack on phen end

B2)bottom side attack, Br attaches first to phen side, then backside attack on COOH end

***The two possible syn attacks (T= top, B=bottom)***

T) both Br attack top simultaneously

B) both Br attack bottom simultaneously

**(2)Table of stereo outcomes : tabulate final stereo assignments of products**

**Anti attack a b Syn attack a b**

T1 R S T R R

T2

B1 B

B2

mp range 200-205 C mp range 90-95 C