Supplementary Information (SI) for Chemistry Education Research and Practice.

Electronic Supplementary Information

for

Utility of creative exercises as an assessment tool for revealing student conceptions in organic chemistry

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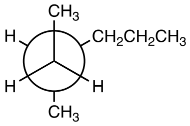
CE1 Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

Fig. S1 Prompt Provided for CE1

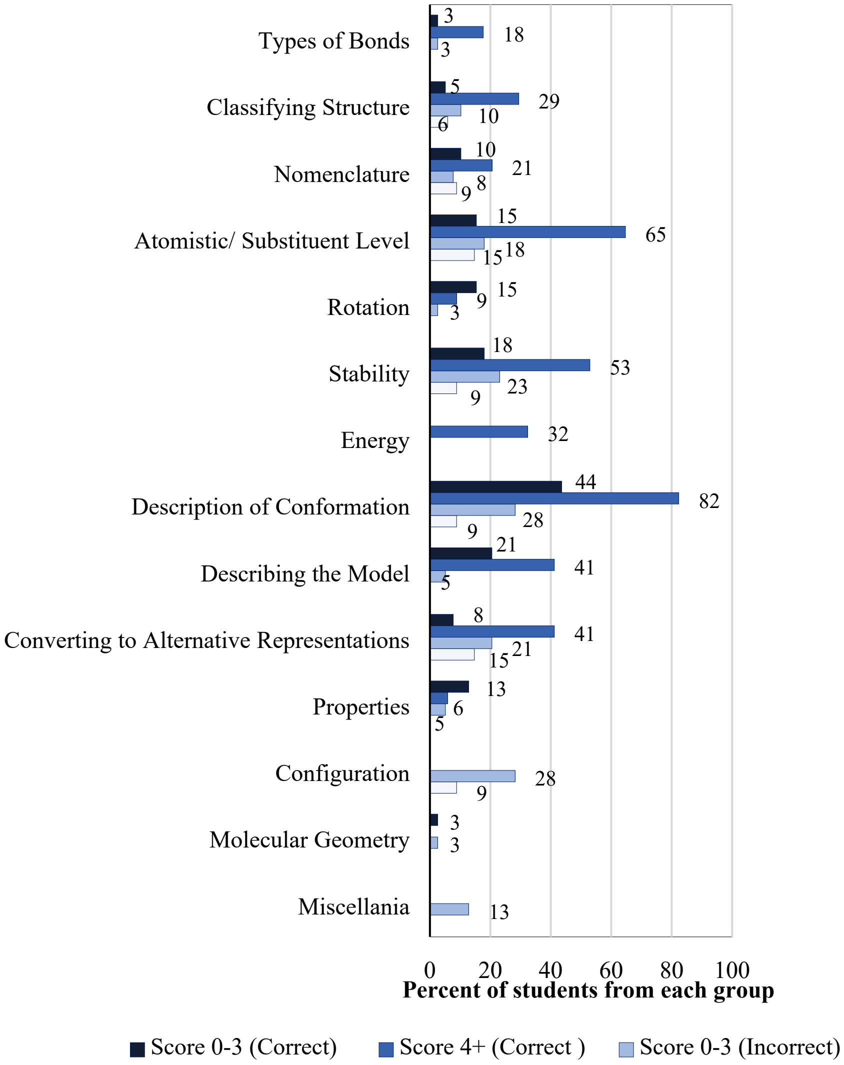
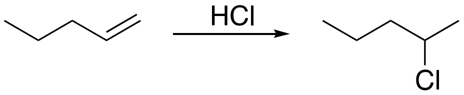


Fig. S2 Percent of respondents in each group, score of zero to three or four or more, who addressed each topic for CE1

CE2 Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

Fig. S3 Prompt Provided for CE2

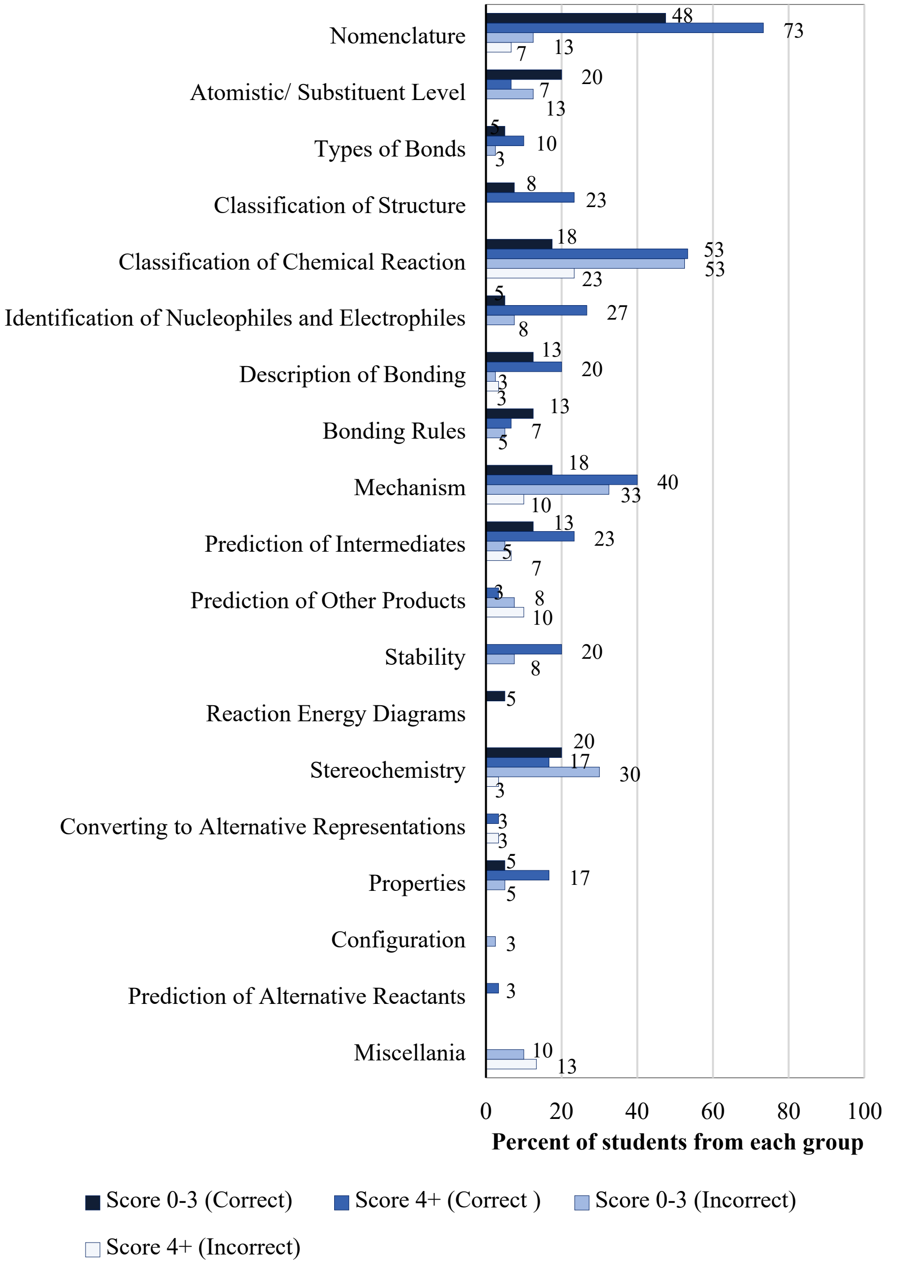
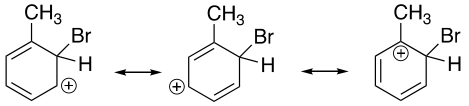


Fig. S4 Percent of respondents in each group, score of zero to three or four or more, who addressed each topic for CE2

CE3 Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



A **B** **C**

Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

Fig. S5 Prompt Provided for CE3

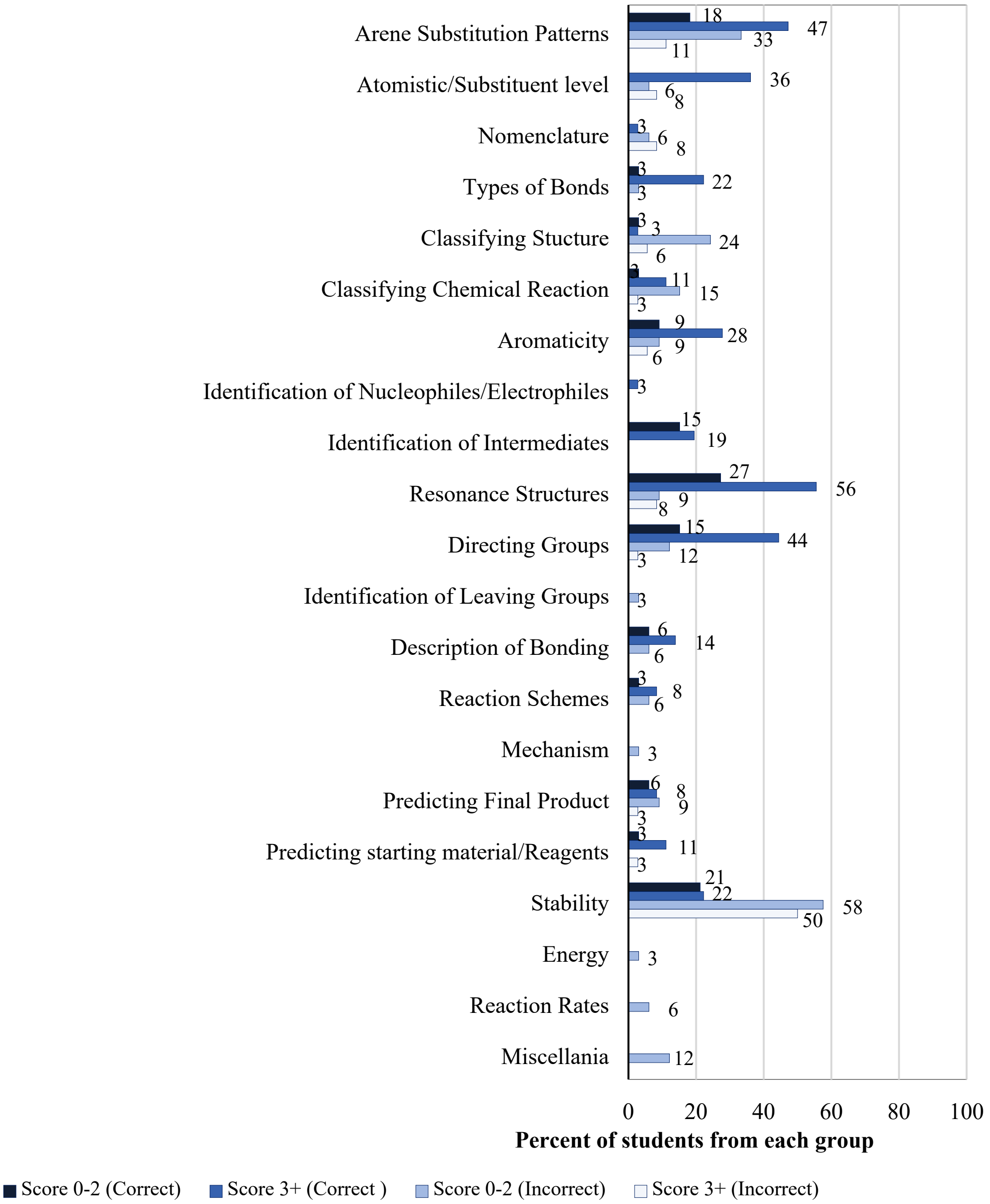
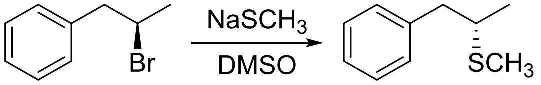


Fig. S6 Percent of respondents in each group, score of zero to two or three or more, who addressed each topic for CE3

CE4 Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

Fig. S7 Prompt Provided for CE4

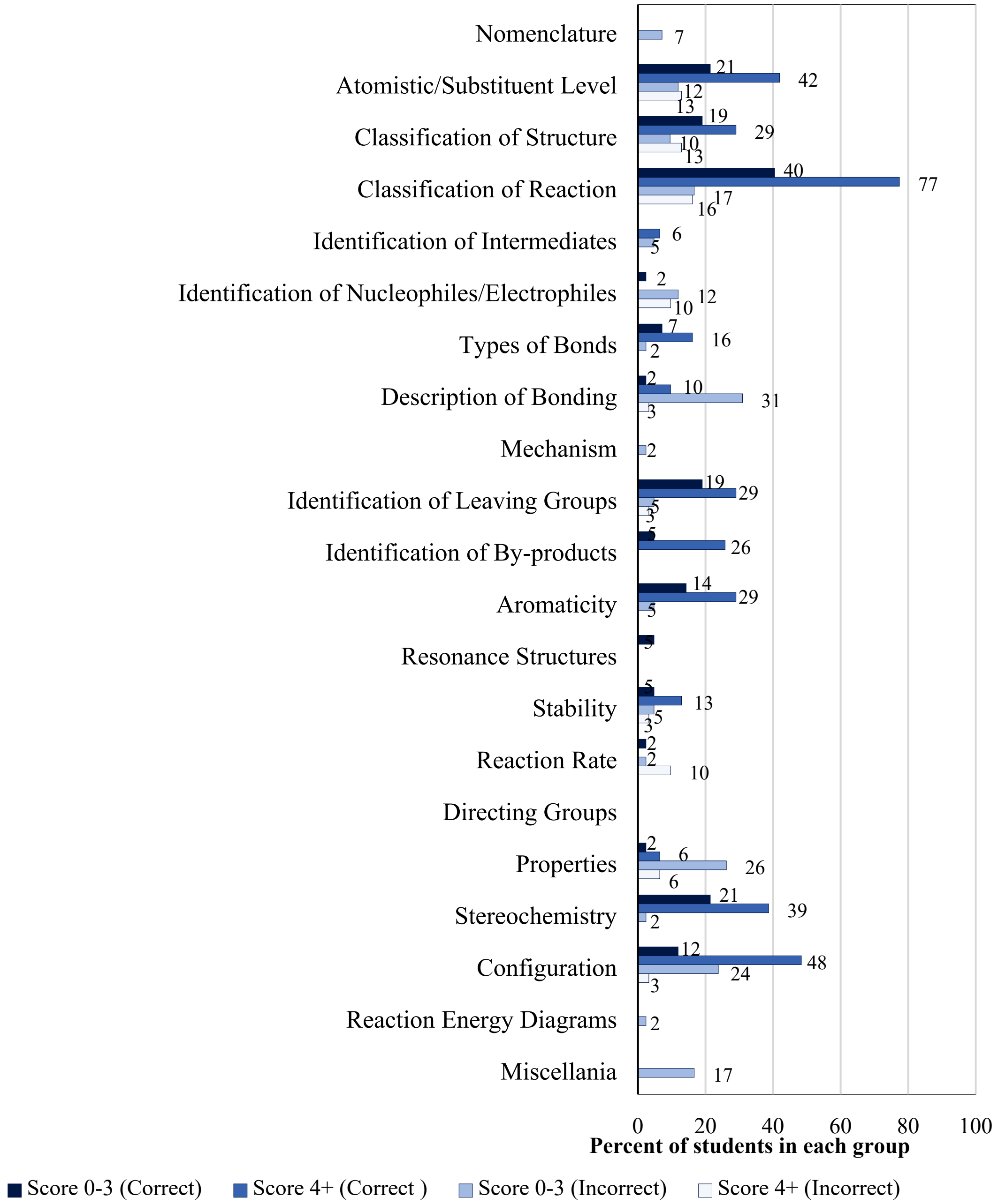


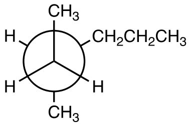
Fig. S8 Percent of respondents in each group, score of zero to three or four or more, who addressed each topic for CE4

Response Classification for Each CE

Italics – correct; **Bold – incorrect;** ***Bold/italics – irrelevant; Bold/Italics/Underlined - unclassifiable***
Values reported in brackets are number of students
Values reported in parenthesis are assigned student code numbers

Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

Creative Exercise 1

Structure

[11] Types of Bonds

[2] Molecule contains single bonds that are able to rotate (51, 75)
[2] The molecule is made up of all sigma bonds that are sp_3 hybridized (11, 14)
[1] All sigma bonds (62)
[1] It is saturated (C_NH_{2N+2}) (47)
[1] All valence shells are filled in this molecule (2)
[1] There are 3 pi bonds (32)
[1] Single bonds are made of one sigma bond (13)
[1] There are no pi bonds in this molecule (9)
[1] This molecule contains no double or triple bonds (single bonds only) (14)

[20] Classifying Structure

[10] The molecule is an alkane (2, 6, 9, 20, 25, 36, 42, 47, 49, 60)
[2] The parent group is hexane (9, 61)
[2] Diagram depicts a branched alkane (20, 75)
[1] There are 7 carbons therefore making it a heptane (17)
[1] This would make this a heptane as 7*2 = 14 + 2 =16 (53)
[1] Butane molecule (65)
[2] Pentane family – 5 carbons (8, 29)
[1] This molecule is a cyclohexane (32)

[18] Nomenclature

[12] Its IUPAC name is 3-methylhexane. (11, 13, 14, 25, 27, 31, 38, 41, 47, 62, 76, 77)
[1] Its name is cis-3-methylhexane. (20)
[2] The IUPAC name for this molecule is 2-ethylpentane. (26, 28)
[1] The name for this molecule is 1,2-methyl-1butylethyl. (22)
[1] The IUPAC name is 2-($CH_2CH_2CH_3$)butane. (65)
[1] Its name is cis-3-methylhex-2-ene. (55)

[1] Stereochemistry

[1] Has stereochemistry (7)

[66] Atomistic/Substituent Level

[1] The central atom is carbon (60)
[10] There are 16 hydrogen atoms (10, 14, 20, 22, 34, 46, 54, 67, 75, 78)
[5] There are 7 carbons (11, ***14****, 17,* ***20****,* ***46****)*
[1] Six carbons in main chain the other a substituent of the chain (11)
[2] Has a 6 carbon chain (15, 53)
[10] Assigned chemical formula as C_7H_{16} (15, 17, 21, ***22****, 25, 36, 47, 53, 63, 76)*
[4] The molecule has 7 sp3 hybridized carbons present (28, 31, 38, 76)
[1] All carbons have sp3 hybridized orbitals. (13)
[1] The structure has one propyl group and two methyl groups (45)
[6] Molecule has 2 methyl groups attached to it (10, 22, 50, 60, 63, 78)
[2] The molecule contains a propyl substituent (46, 63)
[1] There is a propyl group branching off the parent chain (36)
[2] Alkane = $C_NH_{(Nx2)+2} \rightarrow C_7H_{(7x2)+2} \rightarrow C_7H_{16}$ (25, 36)
[1] It has 0 sp2 hybridized carbons and 0 sp hybridized carbons present (38)
[1] Assigned chemical formula as C_5H_{12} (1)
[1] Assigned formula as $CH_3CH_2CH_2CH_2CH_3$ (8)
[1] There are 15 hydrogens (52)
[2] There are 6 carbons (23, 52)
[4] Molecule contains a total of 5 carbons (34, 54, 75, 78)
[1] Molecule has 1 butyl group attached to it (22)
[1] It is an sp orbital (30)
[1] There is only one sigma bond on this molecule (30)
[1] There are two sp2 hybridized carbons present (10)
[1] There are 6 sp hybridized carbons present (10)
[1] There are a total of 23 sp3 orbitals (20)
[1] Assigned formula as $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$ (17)
[1] There are hybridized carbons present (36)
[1] The molecule only has carbons and hydrogens (14)
[1] The shortest possible molecule would equal C_7H_{16} (36)

[16] Rotation

[1] Has different conformers for it (33)

*[8] **Student correctly drew molecule in another conformation (5, 8, 15, 16, 20, 38, 43, 58)*

[5] Molecule contains single bonds that are able to rotate (8, 18, 42, 51, 75)

[1] Molecule rotates around bond between carbons 4 and 5 (15)

[1] The molecule can be in any position (38)

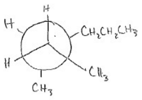
Thermodynamics

[45] Stability

[2] Steric strain between adjacent CH_3 and $CH_2CH_2CH_3$ substituents (6, 18)

[4] The molecule is not in most stable position (19, 46, 54, 62)

[2] A conformer of this molecule would look like (this form is less stable than the one above) (43, 57)



[9] Staggered is more stable than eclipsed (3, 4, 6, 10, 17, 39, 53, 57, 58)

[1] There is more steric than torsional strain here (3)

[2] There is steric strain, especially among the CH_3 and $CH_2CH_2CH_3$ (34, 71)

[1] This molecule would be experiencing steric strain (28)

[1] It would be more stable if the $CH_2CH_2CH_3$ was in anti-position because it is a larger molecule (49)

[2] It would be more stable if the $CH_2CH_2CH_3$ was in anti-position as larger substituent would be less crowded (8, 15)

[2] The most stable position would be if the $CH_2CH_2CH_3$ was in anti-position (20, 58)

[1] It is unstable because of the CH_3 being so close to the $CH_2CH_2CH_3$ (68)

[1] The conformation shown is in the 2nd most stable conformation (76)

[1] If the back carbon is rotated 60 ° counterclockwise, it is the least stable conformation (41) [1] If the back carbon is rotated 120 ° clockwise, it is the most stable (gauche-anti) conformation (41)

[2] It's a stable molecule (7, 30)

[1] This state is due to torsional and steric strain (74)

[1] It is in a staggered conformation which is most stable (49)

[1] The position of the atoms gives it the least possible toric and steric strain. (51)

[1] The front CH_3 and back $CH_2CH_2CH_3$ are gauche resulting in high torsional strain (48)

[3] It is in the most stable conformation state (18, 29, 74)

[1] Most stable of the isomers (43)

[1] Staggered position has more torsional strain than eclipsed position (17)

[1] It's a stable element (59)

[1] Staggered formation creates torsional strain (23)

[1] There will be a lot of torsional strain (12)

[1] This structure is more stable in the eclipse form. (35)

[1] It is stable (67)

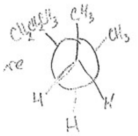
[14] Energy

[7] Staggered is lower in energy than eclipsed (6, 17, 34, 39, 44, 63, 72)

[1] This formation could gain or lose energy if it was rotated to its conformers (5)

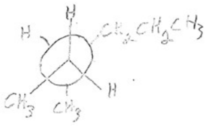
[1] The change in positions creates different levels of strain which changes the energy (44)

[1] This structure has less energy than if the staggered were (5, 45)



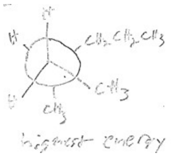
[1] This molecule is not in its highest energy state (14)

[1] The lowest energy conformer is (5)



[1] This structure has a high energy level due to CH_3 and $CH_2CH_2CH_3$ being closer together. (35)

[1] The highest energy conformer is (5)



3-D Conformations

[93] Description of Conformation

[37] The molecule is in staggered conformation (1, 2, 3, 4, 5, 6, 10, 11, 17, 18, 23, 25, 30, 33, 36, 39, 42, 44, 45, 48, 49, 52, 53, 54, 55, 56, 57, 58, 60, 63, 65, 66, 70, 71, 72, 76, 78)

[3] It is currently in gauche conformation (41, 74, 76)

[12] CH_3 and $CH_2CH_2CH_3$ are in gauche position (1, 3, 4, 5, 25, 46, 48, 49, 55, 54, 61, 70)

*[6] The top CH_3 is 60 ° from the $CH_2CH_2CH_3$ (39, **55,** 56, 60, 66, 72)*

[10] Top and bottom CH_3 are anti to each other (3, 4, 19, 48, 49, 55, 54, 56, 61, 70)

*[4] Methyl groups have 180 ° between them. (12, **55,** 65, 72)*

[1] Can have conformational isomers (13)

[1] The front CH_3 and back $CH_2CH_2CH_3$ have a gauche staggered (66)

[2] The molecule is not in the eclipsed position (9, 34)

[1] There is one anti-staggered gauche position in this conformation (9)

[1] The carbon at the 12:00 and the carbon at the 6:00 are in linear conformation (46)

[1] Bond angles are 109 ° (13)

[1] Bond angles are 109.5 ° (60)

[1] The relationship between CH_3 on the back carbon and $CH_2CH_2CH_3$ is anti (70)

[1] The bond angles are all at 60 ° (51)

[1] The front CH_3 and back CH_3 are anti-gauche staggered (66)

[1] One methyl and the only butyl group are gauche to each other (19)

[3] The bond angles are 120 ° apart (32, 36, 71)

[1] The bond angle is 180 °. (30)

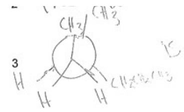
[1] The bond angle between the front CH_3 and back CH_3 is 180 °. (66)

[1] Eclipsed (19)

[1] Methyl groups are in gauche position (12)

[1] The element is staggered (59)

[1] The following is an example of the molecule in a staggered conformation (42)



[1] It is a conformer (38)

[1] This is a conformation (44)

[1] This molecule can conform (31)

[1] 1 gauche, anti-staggered (62)

[25] Describing the Model

[20] This is called Newman's projection (4, 9, 11, 17, 19, 23, 28, 45, 47, 49, 51, 55, 56, 66, 69, 71, 72, 74, 75, 76)

[1] You rotate the bottom half to create different conformations (35, 44)

[1] This projection is the one that looks at the molecule from one and over the main carbon-carbon bond (35, 51, 57)

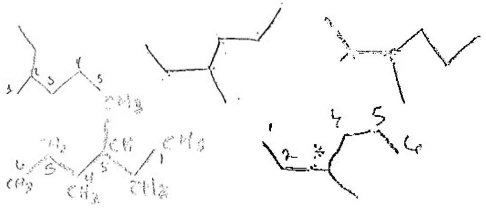
[1] Conformers are easy to be found using this model because it is simply rotating (35)

[1] Shown in the face of a sawhorse model (67)

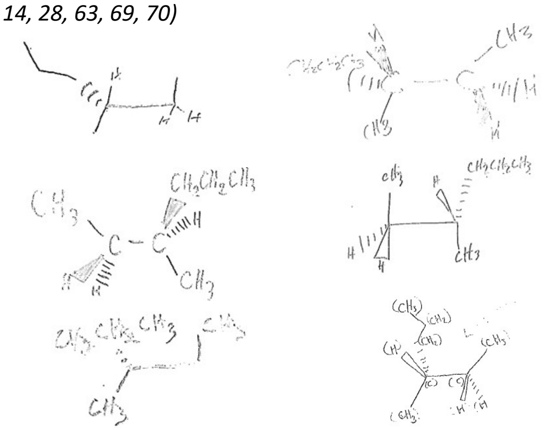
[1] It is a seahorse model (58)

[39] Converting to Alternative Representations

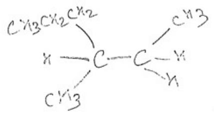
*[10] **Correctly redrawn using a line structure (11, 13, 14, 20, 26, 27, 28, 47, 57, 76)*



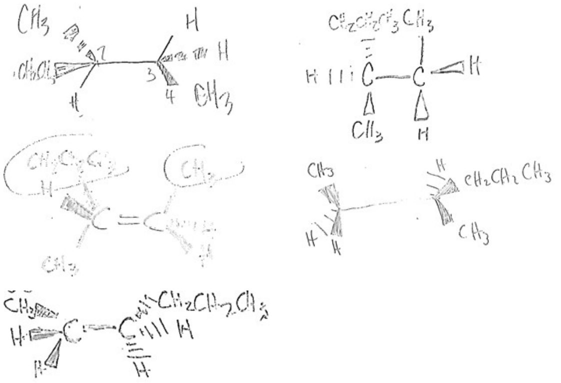
*[7]**Correctly redrawn using wedge and dash notation (5, 9, 14, 28, 63, 69, 70)*



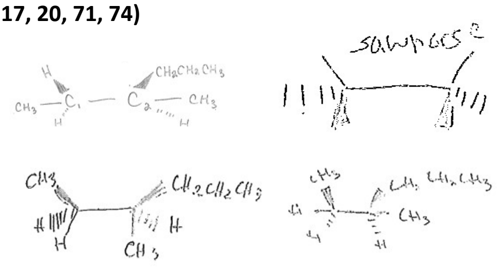
*[4] **Correctly redrawn using a Kekule structure (2, 53, 62, 76)*



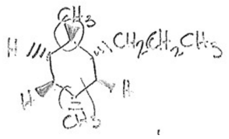
[5] **Incorrectly redrawn using wedge and dash notation (33, 35, 50, 55, 65)



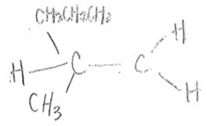
[4] ** Incorrectly redrawn as a sawhorse projection (17, 20, 71, 74)



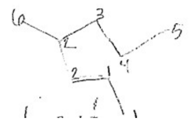
[1] **Incorrectly redrawn using flat ring structure (50)



[1] **Incorrectly redrawn as a Kekule structure (19)

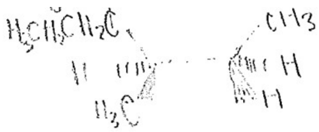


[3] ** Incorrectly redrawn as a line structure (8, 10, 28)

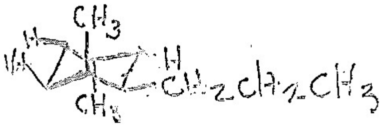


[1] This is the sawhorse projection when viewed from the eye labeled 5. (41)

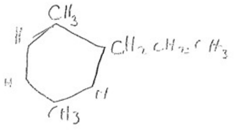
[1] The seasaw diagram would look like (51)



[1] This molecule can be drawn as a chair structure (50)



[1] It can be a cyclohexane if drawn like that (59)



[10] Properties

[1] It would need an extremely strong base to deprotonate it (53)
[1] This molecule is non-polar (2)
[1] This molecule would be a liquid at room temperature (31)
[1] It is liquid at room temperature due to having more than 4 carbons (27)
[2] It is a weak acid (32, 67)
[1] Molecule likely behaves as an acid (65)
[1] This molecule is less acidic than water (2)
[1] It is highly reactive (69)
[1] $CH_2CH_2CH_3$ is the strongest acid (61)

[16] Configuration

[5] It is trans (32, 33, 50, 67, 78)
[4] It is a cis isomer (12, 20, 42, 61)
[1] The two CH_3s are cis (58)
[1] This molecule has a cis bonding structure (31)
[4] It is in a Z formation (5, 42, 53, 70)
[1] Sits at an E – configuration (33)

[2] Molecular Geometry

[1] Tetrahedral shape (29)
[1] The original molecular geometry is sawhorse. (71)

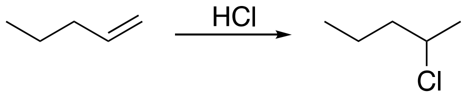
[12] Miscellanea

[1] They are stereoisomers. (12)
[1] It would have the most torginal strain when it moves to the boat position (59)
[1] It is in chair formation (7)
[1] Both the CH_3 are more electronegative then the $CH_2CH_2CH_3$ (18)
[1] Constitutional isomer (moving atoms) (59)
[1] The Anti-methyl groups are [unreadable] to the same carbon (12)
[1] Evenly placed (40)
[1] Balanced (40)
[1] If linear C_NH_{2N+2} (29)
[1] If cyclo C_NH_{2N} lose 2 H because of the circular shape (29)
[1] Is an isomer (7)
[1] Is not in resonance form (7)

Creative Exercise 2

Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

[82] Nomenclature

[29] The starting molecule’s name is pent-1-ene (4, 5, 8, 11, 13, 14, 15, 16, 17, 19, 20, 22, 25, 31, 33, 38, 41, 42, 45, 50, 51, 55, 57, 59, 60, 65, 70, 77, 79)

[6] Reactant is 1-pentene (2, 27, 46, 54, 71, 74)

[34] The product is 2-chloropentane (4, 5, 8, 11, 13, 14, 15, 16, 17, 19, 21, 22, 25, 27, 29, 30, 31, 33, 36, 42, 45, 46, 50, 51, 55, 56, 57, 58, 59, 60, 61, 65, 71, 74)

[4] The other starting material is hydrochloric acid (14, 15, 27, 74)

[1] The starting material is pent-2-ene (30)

[1] The product molecule’s name is 2-chloralpentane (38)

[1] The product is (S)-2-chloryl-pentane. (26)

[2] The product is (R)-2-chloropentane (63, 70)

[1] The product is called 1-chloropentane (20)

[1] The product is 4-chloro-pentane (53)

[1] (E)-1-chloropentane is the product (10)

[1] The pent-1-ene react with HCl (79)

[23] Atomistic/Substituent Level

[1] Cl is 2° (52)

[3] Cl is connected to a secondary carbon (29, 32, 74)

[4] Both compounds have 5 carbons. (15, 22, 34, 67)

[1] Reactant has 5 carbons (32)

[1] The chemical formula is $C_5H_{11}Cl$ *(53)*

[1] There is one methyl group in the first molecule (78)

[1] The starting compound has 11 hydrogens (32)

[1] There are two ethyl groups in the second molecule (78)

[1] Cl attaches to a 3° carbon (8)

[1] The substitution takes place on a 2° section of the molecule (5)

[1] There is only one off branch present (67)

[2] Cl is a halogen (49, 72)

[1] The starting compound has 10 hydrogens (34)

[1] The ending product has 1 chlorine (22)

[3] The ending product has 11 hydrogens (22, 32, 34)

[7] Types of Bonds

[3] It contains one pi bond (double bond) (34, 49, 60)

[2] The product is composed of all sigma bonds (2, 6)

[1] There is a tertiary bond (67)

[1] HCl is bonded with a covalent bond (25)

[14] Classification of Structure (Reactant/Product)

[6] The reactant is an alkene (6, 17, 41, 47, 60, 66)

[2] Product is an alkane (17, 60)

[3] It starts out as pentene (32, 58, 61)

[3] Product is an alkyl halide (47, 55, 75)

[59] Classification of Chemical Reaction

*[11] This is an addition reaction (9, **20**, **28**, 45, 49, 50, 51, 57, **62**, **65**, 76)*

[1] + HX addition (63)

[6] This is a hydrohalogenation reaction (2, 3, 49, 51, 62, 75)

[1] Halogenation reaction (13)

[1] This is a hydrochloronation reaction (14)

[3] It will be an exothermic reaction (19, 28, 81)

[1] The reaction seems to be an acid-base reaction (45)

[5] 2-step reaction (2, 21, 26, 27, 76)

[1] It is an electron rearrangement (81)

[1] A substitution takes place between the reactant and the product (20)

[1] Nucleophilic substitution (53)

[12] It is SN$_2$ substitution (10, 18, 19, 25, 28, 29, 33, 38, 56, 61, 62, 70)

[2] This is an SN$_2$ because it is only one step (1, 59)

[3] This is a one-step reaction (33, 56, 71)

[6] This is a SN$_1$ substitution (5, 8, 46, 55, 65, 66)

[1] It is an endothermic reaction (36)

[2] Reaction is a hydration reaction (16, 26)

[1] Beta-elimination reaction (75)

[18] Identification of Nucleophiles/Electrophiles

[1] HCl is an electrophile (6)

[7] Chlorine is acting as the nucleophile (4, 8, 10, 14, 20, 21, 28)

[1] Cl^- *is a good nucleophile (51)*

[1] H^+ *is the electrophile (21)*

[1] The H is the electrophile (20)

[3] The alkene is a nucleophile (6, 47, 66)

[1] 1-pentene is an electrophile (54)

[1] HCl is a nucleophile (54)

[1] HCl is a weak nucleophile (5)

[1] Cl is the electrophile (77)

Bonding

[16] Description of Bonding (Breaking/Forming)

[2] Adding HCl to the starting group breaks the pi bond (30, 32)

[1] Pi bond breaks forming a positive position in the 2 position. (25)

[1] The reaction between electrophile and nucleophile to form new covalent bond (39)

[1] In the reaction of alkene, pi bond is broken and, in its place, sigma bonds are formed (39)

[1] pi bond broken to form a new single bond (75)

[1] Nucleophile (Cl^-*) is reagent that donates unshaired pair of electrons to form the new covalent bond (39)*

[1] The chlorine bonded to the most stable carbocation (41)

[1] Double bond breaks when HCl added (19)

[1] The double bond breaks in this reaction (13)

[1] The first step is the pi bond breaking (46)
[1] Carbon double bond goes away (58)
[1] HCl is also breaking its bond, separating H and Cl so that HCl is not in the products (47)
[1] The double bond breaks in this reaction, forming a bond with Cl (47)
[1] The breaking of bond to make stable ion or molecule (39)
[1] The double bond relocates (67)

[9] Bonding Rules

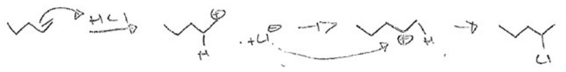
[1] Cl will bond to the carbon with the least amount of hydrogen bonds (35)
[1] Cl will always bond to the more substituted carbon (36)
[1] The hydrogen will attach to the carbon on the end because it has the most hydrogens when the double bond is broke (54)
[1] This follows Markovnikov's principle, H adds to the rich side (3)
[1] This follows Markovnikov's rule, Cl is added to the most substituted carbon (9)
[1] This reaction follows Markovnikov's rule (48)
[1] This is a Markovnikov reaction (41)
[1] The Cl is happy because it is attached to the bottom of where the double bond was (61)
[1] Doesn't have regioselectivity (18)

Mechanism

[9] Complete Mechanism

[2] This reaction will form a carbocation (18, 48)
[1] This is a multistep reaction, where first the double bond breaks and a + charge appears. (66)
[1] The reaction has 2 steps, the protonation of the substrate and the chloronation of the substrate (14)
[1] Reaction takes place via 2 steps, first leaving group leaves and creates a carbocation intermediate, then secondly the halogen attaches to the carbocation (55)
[1] The positive charge moves from being a primary to a secondary. (66)
[1] No rearrangement will occur due to it already being most stable at 2°, no option for 3° (3)
[1] **(1)**

[1] The arrows would push like this: (20)



[17] First Mechanistic Step: Addition of Electrophilic H^+

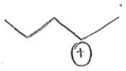
[1] The first step, the hydrogen adds to end of chain breaking double carbon (74)
[1] The H becomes an H^+ and takes the double bond's electrons and gives the 2nd carbon from the right a + (18)
[1] The H^+ breaks the double bond resulting in formation of carbocation (15)
[1] Hydrogen from HCl breaks the double bond (17)
[2] The hydrogen gets rid of the double bond (56, 61)
[1] Addition of the H molecule gets rid of the double bond (33)
[1] The hydrogen on HCl connects to the carbon on the end of the double bond (58)
[1] The pie bond of the starting material is broken and its electrons are transferred to H of HCl. (11)
[2] The double bond gets protonated in the reaction (13, 14)
[1] This reaction involves protonation of 1-pentene by HCl. (2)
[1] In the first step of this reaction the H^+ from HCl reacts with the double bond of the first molecule and Cl^- is left off (42)
[1] HCl will donate its proton to the right side of the double bond which will then break (48)
[1] *(73)*

[1] The hydrogen helps break the double bond (72)
[1] Chlorine breaks the double bond (31)

[10] Second Mechanistic Step: Addition of Cl^-

[1] HCl splits leaving H^+ and Cl^-. Cl^- moves in and bonds to positive charged C (15)

[1] The Cl^- formed from protonating the starting materials bonds with the carbocation to form the product. (11)
[1] After the double bond is removed, before the Cl is added the molecule has a positive charge on it (72)
[1] The chlorine is attached where it is to get rid of the charge and make molecule neutral (56)
[1] The Cl is a – after the H splits off and it bonds with the + on the carbocation (18)
[1] The nucleophile attacks the plus charge in the molecule to make the product (4)



[1] During the 2nd step, Cl bonds to C_2 (76)
[1] *(73)*

[1] Cl takes over the electrons from the broken double bond (30)
[1] The bridging intermediate blocks off the one side of the molecule so that is why the Cl had to bond on the bottom (49)

[9] Incorrect Mechanistic Steps

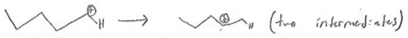
[1] 

(73)

[1] When the double bond is broken, the carbons are left with positive charges. The hydrogen bonds with one of the carbons, eliminating one of the positive charges. When hydrogen breaks from Cl, it leaves Cl with a negative charge. Cl bonds with the other positively charged carbon (35)
[1] The alkene breaks to an alkane leaving excess charges so HCl can bond to it (9)
[1] The double bond is removed to a charge, then Cl is added on (52)
[1] First step in reaction is to break double bond, leaving an electron poor spot for the Cl to attack as it has a negative charge on it (3)
[1] The double bond is broken with HCl creating a H_2 molecule and Cl^-.The Cl^- is attached then after to the 2nd carbon on the chain (22)
[1] The pi bond, where there is a double bond, breaks. This breakage creates a plus charge at the 2nd carbon. The negative Cl forms a bond with the plus charge (79)
[1] This is a multi-step reaction where first the double bond breaks and positive charge appears. After the first step of breaking the double bond, we have a carbocation. Carbocation rearranges the positive charge before the Cl^- attacks to be more stable (66)
[1] First step is to break the double bond (81)

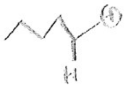
[18] Predicting Intermediates

[10] The following is the intermediate step (15, 16, 38, 41, 48, 58, 63, 72, 73, 76)



[1] (21)
[1] Before chlorine bonds, there is a second degree (2°) carbocation in the intermediate (41)
[1] After the first step of breaking the double bond we have a carbocation (66)
[1] Intermediate A will be a 2°, intermediate B will be a 3° carbocation (81)

[1] It creates a bridging intermediate (49)
[1] There will be 2 intermediates (81)



[1] This reaction wouldn't have any intermediates (50)
[1] The intermediate carbocation will likely look like (6)

[6] Prediction of Other Products

[1] A minor product could be 1-chloropentane (27)
[1] A positive H^+ molecule is a byproduct of the reaction (46)
[2] No minor products (25, 31)
[1] There could be a product where Cl is on another carbon

[student drew examples illustrating on C1 or C3] depending on if the carbocation relocates and where it relocates to (41)
[1] An expected product may be but it's not because with Cl being attached to a 2° carbon is more stable than 1° carbon (20)

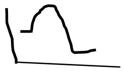
[11] Stability

[2] More substituted carbocation are more stable (20, 39)
[1] Cl bonds to carbon 2 because it's 2°, whereas carbon 1 is 1°, 2° is more stable (76).
[1] The carbocation will form on the 2° carbon because it is most stable (11)
[2] The final product is more stable (2, 74)
[1] A stable reaction because of the location of the Cl (53)
[1] In this form, the reactant is most stable (32)
[1] The product is a 2°, making it more stable than the reactant (1)
[1] The addition of HCl makes the product less stable than the reactant (33)
[1] The reaction is stable (67)

[2] Reaction Energy Diagrams

[1] Its energy diagram should look like the energy diagram below where the arrow labeled b indicates the rate determining step and the middle, labeled A is the intermediate step (38)

[1] The graph would be exothermic, as energy of products is lower than energy of reactants (1)



[33] Stereochemistry

[7] The product contains a stereogenic carbon (54, 55, 62, 63, 70, 71, 78)

[3] The starting material contains zero stereogenic carbons (30, 63, 70)

[1] If the H is facing down it would be R. If the H was facing up it would be S. Using Cl as our stereochemistry (59)

[1] The Cl group is not stereospecific as it can go either on the front or the back (3)

[3] The product is chiral (28, 55, 65)

[1] Product contains 0 planes of symmetry (55)

[1] There is no plane of symmetry (52)

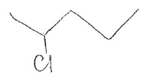
[1] There are no stereogenic carbons in the product (30)

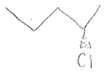
[6] The stereogenic carbon has an R configuration (46, 54, 62, 63, 71, 78)

[1] This molecule is chiral (31)

[1] Chiral (29)

[1] Both molecules are chiral (56)

[1]  **would be the enantiomer/mirror image for the product (10)**

[1]  **would be a diastereomer for the product. (10)**

[1] Product is achiral (8)

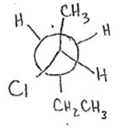
[1] Enantiomers (29)

[1] The molecule is stereogenic (7)

[1] It's non-meso. (50)

[1] Converting to Alternative Representations

[1] This is another projection of the product (57)



[10] Properties

[4] HCl is a strong acid (15, 34, 42, 57)

[1] HCl is an acid (78)

[1] The reaction occurs in an acid (hydrochloric) (14)

[1] This wouldn't require a catalyst because the HCl is strong enough to break bonds (50)

[1] HCl also acts as a catalyst (36)

[1] pent-1-ene acid acts as a base and accepts electrons (77)

[1] It would react poorly with an alcohol (53)

[1] Configuration

[1] Compound formed is sys or trans, doesn't matter because it takes two steps so arrangement happens. (9)

[2] Predicting Alternative Reactants for Class of Reactions

[1] The starting material could undergo similar reactions with other molecules consisting of a hydrogen bonded to a halide (70)

[1] The reaction could also take place with NaCl instead of HCl (70)

[12] Miscellanea

[1] The double bond on the reactant molecule has HCl added to its molecule to give the molecules more electrons (45)

[1] The pi bond is a source of electronegativity; H^+ and Cl^- add to the C_5 that had a double bond. They don't add anywhere else (9)

[1] The carbocation is the Cl^- (59)

[1] HCl is used well with SN_1 reactions due to its H; SN_1 react well with O and H substrates (17)

[1] The molecule is deprotonated (36)

[1] The product molecule could be arranged as 1-chlorocyclopentane (55)

[1] A five carbon chain reacts with HCl (75)

[1] The conjugate base of HCl is Cl^- (42)

[1]  ***and HCl are the starting products (58)***

[1] Chlorine is bonded to the second carbon on the product's side (60)

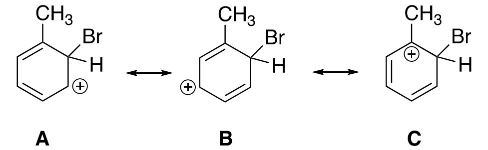
[1] There are no carbocations present (7)

[1] H^+ deprotonates (4)

Creative Exercise 3

Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



A B C

Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you

[44] Arene Substitution Patterns

[6] The Br and H are in the ortho position in relation to the CH_3 (5, 22, 25, 49, 72, 75)
[1] Substituents are in ortho arrangement (32)
[3] CH_3 and Br in are in ortho position (42, 55, 62)
[2] Structures above reflect ortho (38, 39)
[3] All molecules are in the ortho position. (28, 34, 78)
[1] They are in ortho position (61)
[2] These molecules are in the ortho position, which is 1,2 (4, 17)
[1] Br is in the ortho position (1:2) (48)
[1] This reaction will want to maintain an ortho or para, and is in the ortho (1)
[1] The carbocation is in ortho and para to the carbon attached to Br and H (53)
[2] This reaction would give a product that is ortho… 1,2 orientation (3, 33)
[1] Ortho (15)
[1] It's ortho (52)
[1] In A, the proton is ortho to Br (77)
[1] B, [the proton] is para, (77)
[1] C, [the proton] is in meta position (77)
[1] It is a meta (67)
[1] A, B, and C are all in the para position (14)
[1] The CH_3 and Br are meta (18)
[1] Structure A shows an ortho position of the + charge (51)
[1] Structure B shows a meta position of the positive charge (51)
[1] For A and B, the plus charge is in the meta position (74)
[1] Br and H are in the ortho stage on each molecule (30)
[1] A, B, and C are all ortho products (16)
[1] This is an ortho product (35)
[1] From "ABC" it goes: para, meta, ortho. (46)
[1] A has Br in the ortho position (76)
[1] The Br in structure B is in ortho position (12)
[1] Br and H remain in the ortho position (74)
[1] Para, bond (26)
[1] A,B,C don't like meta. (29)
[1] The position of the substituents always remain unchanged when this molecule is produced (36)

[28] Atomistic/Substituent Level

[1] They all have the same amount of electrons (61)
[2] The CH_3 is called a methyl group (4, 34)
[2] There is one methyl group attached to the molecule (60, 78)
[3] It contains 7 carbon atoms (11, 14, 49)
[1] There are 8 hydrogen atoms in this molecule (32)
[1] Halogen and methyl substituents (19)
[3] Each molecule contains a six carbon ring (11, 34, 60)
[1] They all have bromine on carbon number one (60)
[1] They are all carbocations (11)
[1] They all have carbocations (47)
[1] Each is a charged carbocation (75)
[1] The positive charge is on a tertiary carbon in C (76)
[1] The carbon attached to bromine is a secondary carbon (32)
[1] H's attached carbon is 3° (52)
[1] Br's attached carbon is 3° (52)
[1] Br has a 3° substitution (4)
[1] CH_3's attached carbon is 2° (52)
[1] Each molecule is a tertiary structure (17)
[1] The carbocations are all on different carbons in each molecule (47)
[1] Each contains a 3° Carbon (75)
[1] Carbocation (62)
[1] The positive charge placements are due to the bromine (56)

[5] Nomenclature

[1] Product molecule is named 2-bromotoluene **or 2-bromo-1-methylcyclohexane (55)**
[1] The IUPAC name for A is 1-bromo-2-methylcyclohex-2,4-ene (38)
[1] The actual chemical name is 1-bromo 2 methylcylohexene (46)
[1] The IUPAC name of this structure would be 1-bromo, 2-methyl, 2,5-cyclohexene (28)
[1] 1-methyl-6-bromo-cyclohex 1,3 ene (26)

[11] Types of Bonds

[1] It has two pi bonds, and the + occupies another pi orbital (49)
[5] Each structure has two pi bonds (14, 15, 22, 60, 75)
[1] There are four carbons with pi bonds (13)
[1] Each molecule above has 2 double bonds (34)
[1] The double bonds must alternate with single bonds (35)
[1] The double bonds are made up of a pi bond and a sigma bond (57)
[1] Electrons in pi bonds are in p orbitals (13)

[13] Classification of Structure

[1] All of the molecules have benzene rings as the parent (51)
[1] It's a benzene ring like molecule (18)
[1] It is a hexane (67)
[1] It has a cyclohexane base structure (69)
[1] The parent ring is cyclohexane (74)
[1] They all have a cyclohexane ring (10)
[1] Molecule is a cyclohexane with substituents (45)
[2] Represent alkenes (60, 75)
[1] Each molecule has 6 carbons, making it a cyclohexadiene (17)

[1] Each molecule is classified as an alkene, which is characterized by the double bond. (17)
[1] The parent chain in this molecule is a hexene ring. (36)
[1] Is an alcohol (7)

<u>[12] Classification of Chemical Reaction</u>

[2] The three molecules are the possible intermediates for an electrophilic substitution reaction (51, 53)
[2] This is an electrophilic substitution reaction (11, 25)
[1] In a E_AS, this reaction is synthesized by $Br_2/FeBr_3$ (63)
[1] This molecule could undergo E1 substitution reaction. (31)
[1] Sn1 or E1 could be used for a reaction (29)
[1] This isn't an electrophilic substitution because the double bonds are moving (64)
[1] This is an SN_1 reaction (48)
[2] E1 elimination (19, 39)
[1] This molecule could go through an elimination reaction. (35)

<u>[18] Aromaticity</u>

[10] All of these structures are not aromatic (8, 15, 18, 28, 29, 36, 47, 62, 70, 78)
[1] None of these are aromatic products (16)
[1] This is not an aromatic ring as there are four electrons in the pi bond in each (79)
[1] It is not aromatic because there is not a pi orbital on every atom (49)
[1] These structures are not all aromatic (61)
[1] Aromatic molecule (65)
[2] These are aromatic molecules (10, 71)
[1] The molecule(s) are aromatic ($6\pi\ e^-$) (55)

<u>[1] Identification of Nucleophiles/Electrophiles</u>

[1] They are all electrophiles (11)

<u>[15] Identification of Intermediates</u>

[2] The three molecules are the possible intermediates for an electrophilic substitution reaction (51, 53)
[1] The three diagrams are all carbocation intermediates due to resonance (54)
[1] Three arrangements of a carbocation intermediate are shown (55)
[1] The structures are carbocation intermediates (42)
[4] A, B, and C are all intermediate resonance structures (30, 33, 65, 76)
[2] Shows the intermediates (11, 27)
[1] They are intermediates to a reaction (10)
[1] Three intermediates of a two step reaction (25)
[1] A, B, and C shows the transition state of Br being added to 

(20)
[1] Structures A, B, and C are all interchangeable intermediate steps to a reaction (38)

<u>[38] Resonance Structures</u>

[3] Structures A, B, and C are all resonance forms (26, 38, 42)
[4] It is a resonance structure (49, 53, 57, 71)
[4] These are all forms showing different possibilities of resonance in the structure (3, 14, 28, 74)
[1] The diagram shows different resonance structures (78)
[4] A, B, and C are all intermediate resonance structures (30, 33, 65, 76)
[1] This shows a resonance structure from the charge moving around, charge is being shown that is not in one spot. (82)
[1] These are three different resonance forms for benzene derivatives (9)
[1] The charge is moved around via resonance (72)
[1] Has resonance/charge moves around ring (15)
[1] Positive charge is delocalized throughout ring (19)
[1] Shows how the (+) is spread out through resonance (11)
[1] The molecule may change from A $\rightleftarrows$ *B and B* $\rightleftarrows$ *C, but not A* $\leftarrow$ *C (36)*
[1] Each picture is a depiction of where the charge could be at any point in time (19)
[1] Each of the three intermediates represents a different arrangement of pi bonds (25)
[1] The resonance structures show the ability of the molecule to spread out the charge, making the molecule more stable (57)
[1] The molecules show resonance, which helps stabilize the molecule (17)
[1] A, B, and C are all the same compound with different arrangements of the + charge but the same chemical formula (79)
[1] Each one of these is a different version of the same molecule (47)
[1] The ↔ arrow is not a reaction arrow, but instead is to show different forms. (71)
[1] The electron can delocalize (18)
[1] The carbocation is moving to different carbons making it more positive than the others (45)
[1] The cation moves based on stereochemistry/resonance (69)
[1] The plus signs indicate the different resonance structures possible (4)
[1] Resonance structures allow halogens to stabilize carbocations (13)
[1] Resonance is what is stabilizing this atom by moving the positive charge around with the breaking and addition of the double bond (22)

[1] The carbon bonds rotate along with the positive charge (78)

[1] Double bonds rotate throughout the molecule (45)

[42] Directing Groups

[13] Methyl group is o, p directing (8, 9, 12, 13, 14, 25, 56, 57, 70, 72, 73, 74, 76)

[1] When CH_3 is attached to a benzene, it typically adds reactants to the ortho or para position. (20)

[6] CH_3 is an electron donating group (8, 12, 13, 32, 35, 66)

[6] CH_3 is activating group (3, 41, 56, 63, 66, 72)

[3] Br is a deactivating group (3, 9, 56)

[1] Br group is ortho-para director (14)

[1] Br is a halogen, but ortho-para directing (56)

[2] Br is electron withdrawing group, but para/ortho directing (8, 13)

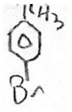
[1] To form this product either the CH_3 or the Br group could have been attached first because they both favor ortho, para positions. (5)

[1] This is an ortho-directed reaction (63)

[1] Br could also have been placed in the para position. (72)

[1] This reaction will want to maintain an ortho or para, and is in the ortho (1)

[1] The bromine could have also added to this location, because activating groups are ortho-para directors. (41)



[1] It prefers the para and ortho directors. (66)

[1] Molecule has an ortho director (45)

[1] Br on the benzene prefers ortho, para (9)

[1] This is an electron donating group due to the CH_3 (1)

[3] Identification of Leaving Groups

[1] Br would be a leaving group in this reaction due to it being a stronger base (1)

[1] Br is the best leaving group for these (61)

[1] The Bromine is the best leaving group, followed by the methyl group. (46)

[12] Description of Bonding (Breaking/Forming)

[2] CH_3 was added to benzene ring first, Br second (54, 70)

[1] A, B, and C can be easily deprotonated (this is a middle step of a reaction that will lead to the molecule being deprotonated to become stable) (14)

[1] The previous step put the Br on (27)

[1] A double bond will form again to stabilize the benzene structure (9)

[1] These groups being added to the benzene ring could have been added in any order, but it makes sense to add CH_3 first, because then adding Br would be faster as CH_3 is an activating group (41)

[1] Formed by the substitution of Br into the ring (62)

[1] A negatively charged chemical could bond to the positive charge and make the benzene ring stable (82)

[1] Alkyl halides can still undergo elimination reaction if they can form stable carbocation (39)

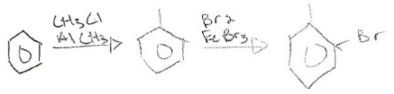
[1] Hydrogen would bond with another H to make H_2 gas or OH to make H_2O. (82)

[1] E1 elimination occurs in two steps (39)

[1] In order to make the alkene into an alkane, the double bond must be broken. (17)

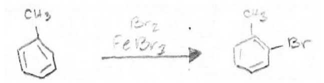
[7] Reaction Schemes

[1] A possible reaction series could be (20)

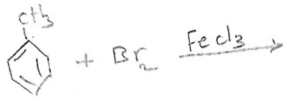


[1] If we started with benzene, the first rxn would be CH_3Cl $AlCl_3$ to add the $–CH_3$ group; second rxn would be Br_2 $FeBr_3$ so the halide joins in the ortho position. (55)

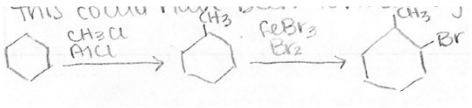
[1] *complete product (63)*



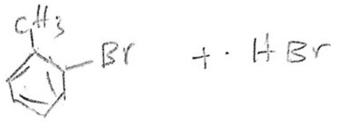
[1] *(73)*



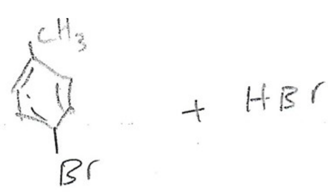
[1] This could have been formed by (1)



[1] (73)



[1] **(73)**

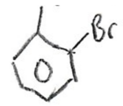


[1] Mechanism

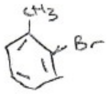
[1] E1 elimination, Breaking C-X bond to form carbocation intermediate followed by the loss of H^+ to form alkene (39)

[9] Predicting Final Product

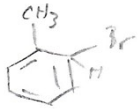
[4] The final product is (14, 48, 67, 70)



[1] The final product would be (notice placement of pi bonds) (20)

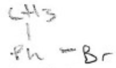


[1] The final product is (54)



[1] These are all 3 possible products of one reaction (35)

[1] Another way to draw the product would be (20)



[1] A and B are the major and intermediate products (52)

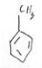
[7] Predicting Starting Material/Reagents

[2] A beginning reactant might be (16, 33)

[1] This is a depiction of the carbocation intermediates formed when bromine is being added to via $Br_2/FeBr_3$ (41)

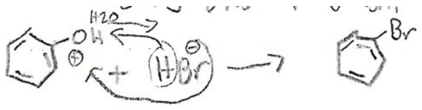
[1] CH_3 was likely (could be) added to the ring using $ClCH_3$ and $AlCl_3$ (57)

[1] Is the product where was used as a reactant (18)



[1] Base was a benzene ring (15)

[1] If the CH_3 wasn't there, the benzene got Br from this reaction (can assume) (82)



Thermodynamics

[70] Stability

[1] Intermediate B is especially stable (33)

[1] A is least stable (77)

[8] C is the most stable (4, 21, 31, 32, 61, 69, 70, 77)

[1] C is the most stable of all. Positive charge to an E donating CH_3 (9)

[1] C is especially stable (26)

[1] C is the most stable of the three in their current state (29)

[1] If this were in a reaction problem, C would be the intermediate that is especially stable (10)

[1] B is not as stable as C due to the + charge location (79)

[16] "B" is the most stable (8, 12, 30, 38, 42, 45, 46, 48, 50, 53, 54, 63, 64, 65, 71, 76)

[1] "B" is the most stable product (16)

[1] Group "B" will be the most stable (5)

[1] Formation B would be the most reactive formation by moving the positive charge away from the cluster of groups (22)

[1] B is not a stable carbocation (47)

[9] Structure C is the least stable form (8, 28, 30, 34, 42, 46, 53, 54, 71)

[2] C is not very stable (27, 62)

[1] C is very unstable and not good to happen. (20)

[1] Structure C is the least stable product (16)

[1] Stucture C would not be stable. You don't want a charge on the CH_3 (82)

[1] Structure C is bad due to the positive charge placed on carbon attached to CH_3 (3)

[1] C is least likely intermediate (65)

[1] Structure C is very unstable, due to stereogenic crowding of the alkyl group and the positive charge (51)

[2] In step C, you have a (+) next to a (+), which is BAD (30, 33)

[1] The letter C is a bad one because the (+) and the CH_3 (+) are together. (66)

[1] C is the most stable configuration because CH_3 is an activating group (41)

[1] C is the most stable because the + charge is close to CH_3 (79)

[1] Configuration C is most stable because it has the + and – charges together (55)

[1] The most stable resonance form would be C due to the (+) being with the (+). (1)

[1] The orientation of "C" will not be a good group to produce and will be very unstable (5)

[1] The product above A is the most stable out of the three forms (20)

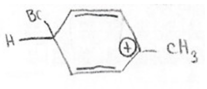
[1] A and B are the stable ones (66)

[1] Formation A would be the most stable formation of this molecule due to the electronegativity of the molecule (22)

[1] No aromatic stability (19)

[1] If iodine replaced bromine, it would increase the reactivity of the molecule. (36)

[1] The most stable form of the three would be in para with the + charge under the CH_3, works for A, B, C (29)



[1] B is not as stable as C due to the + charge location (79)
[1] Carbocation: stability: spread out positive charge (more stable) inductive effect and hyperconjugation (39)
[1] Group "A" will be a stable group, but not the best option (5)
[1] This product would have a higher reactivity than benzene because CH_3 is a stronger activating group than bromine is a deactivating group. (41)

[1] Energy
[1] C has the highest energy (50)

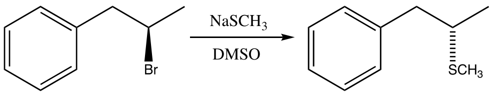
[2] Reaction Rates
[1] Reaction would occur fastest with B as intermediate (65)
[1] CH_3 does react faster and is more reactive than benzene (66)

[6] Miscellanea
[1] C has a double plus charge (67)
[1] The + is rotating clockwise (67)
[1] Has stereochemistry (7)
[1] They all lack three-dimensionality within this given drawing (10)
[1] The low steric hindrance makes it possible for carbocation (12)
[1] If these were intermediates, the order would most likely be C, B, A (50)

Creative Exercise 4

Provided Prompt

Write down five **correct, distinct, and relevant facts** about:



Five (5) statements will get you full credit for the problem, which is worth a total of 5 points. The information you use should be information you learned in chemistry courses.

[4] Nomenclature
[1] The starting material is R-2-bromo-propane attached to a cyclohexene (17)
[1] Hex-3-ene is the main component of both (69)
[1] The first structure is 3-bromylcyclohextane (61)
[1] The second structure is 3-sufocyclohexane (61)

[39] Atomistic/Substituent Level
[3] There are 9 carbons in the first molecule and 10 carbons in the second (41, 55, 78)
[1] There are 9 carbons on the reactants side (60)
[1] There are 9 carbons in the substrate molecule (14)

[1] Both molecules include a carbon ring (34)
[1] Both molecules contain a functional group (34)
[4] SCH_3 is replacing Br (47, 58, 74, 79)
[1] SCH_3 is substituted in place of Br (65)
[1] The bromide is broken off and is replaced with SCH_3 (22)
[1] Bromine was replaced with sulfur, carbon, and hydrogen atoms (33)
[1] Br is a secondary halide (54)
[1] There is only one tertiary carbon found in the product (11)
[1] There is 1 tertiary carbon in each molecule (32)
[3] There is a primary carbon present in each molecule (5, 33, 52)
[1] They could be written as  *(38)*

[1] The molecules can also be rewritten as (45)

[1] Could be drawn (29)

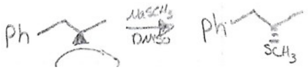
[1] The Br is a secondary (74)
[1] Br is in a secondary position (13)
[1] 2° Br is substituted (62)
[1] The hexcyclo ring doesn't change during the reaction (58)
[1] Both molecules contain 9 carbons (34)
[1] There are 10 hydrogen atoms per molecule (32)
[2] Na has a negative charge (4, 8)
[1] It is placed on a tertiary bond. (67)
[1] There are 6 tertiary bonds (67)
[1] There are no tertiary carbons present (50)
[1] Benzene has chemical formula C_6H_6. (39)
[1] The Na has a + charge (72)
[1] The SCH_3 has a – charge (72)
[1] Br is a halogen (75)
[1] The Br on the original compound stands for Bromine (74)

[26] Classification of Structure

[4] Each molecule on product and reactants contains a benzene ring (32, 56, 67, 78)
[1] The substituents are attached to a benzene ring (71)
[1] The base is a propyl group connected to a benzene (25)
[2] Contains a benzene ring (18, 75)
[1]  *is a benzene ring (4)*

[2] Parent ring is a benzene (60, 65)
[1] Product contains a benzene ring (11)
[1] The molecule that is reacting contains a benzene ring (14)
[1] The cyclic structure on the reactant and product is a phenyl group (31)
[1] The basic compound of this molecule is benzene (22)
[1] Solution and product both contain benzene ring (15)
[1] The propyl is connected to a 6-C ring. (6)
[2] Both molecules have a phenol (Ph) group (38, 41)
[1] Another name for this benzene ring is phenol (9)
[1] Both contain a cyclohexane ring (10)
[1] The parent chain is a cyclohexene molecule (36)
[1]  **is called benzoic acid (79)**

[1] Has a hexcyclo ring on product (58)
[1] Has a hexcyclo ring on reaction (58)



[61]

[1] The R group of the molecule in benzene ring structure (25)

Classification of Reaction

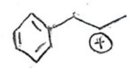
[11] This is an SN_2 reaction. (1, 14, 15, 19, 22, 26, 29, 35, 41, 52, 66)
[9] The reaction is a SN2 substitution (5, 9, 20, 28, 30, 38, 45, 62, 70)
[1] It is an SN2 reaction (nucleophilic substitution) (49)
[2] This is an SN2 replacement reaction (27, 31)
[16] It'll do a substitution reaction. (2, 6, 11, 13, 32, 43, 47, 48, 53, 60, 63, 65, 67, 69, 75, 76)
[1] SN_2 reactions are one-step reactions (41)
[2] The reaction is a replacement reaction (16, 25)
[1] It is an exothermic reaction (36)
[1] A substitution reaction occurs between Br and SCH_3 (36)
[1] Electrophilic substitution reactions (like this) are used for alkyl halides (51)
[1] This is an electrophilic substitution reaction (51)
[4] This is an SN1 reaction (16, 55, 56, 60)
[1] This is a SN_1 reaction (substitution) that involves an electrophile. (50)
[1] This can be done by Sn1 or E1 reaction (12)
[1] This is an E1 reaction (2 step) (46)
[1] This is not an equilibrium reaction (38)
[1] This reaction would also be an E_2 reaction as it is a one-step and the Br and SCH_3 are secondary (1)
[1] At Br and SCH_3 a addition reaction could be done (29)
[4] The reaction is a substitution reaction (20, 28, 45, 62)
[1] This is not an elimination reaction (74)

[4] Identification of Intermediates

[1] No intermediate carbocation is formed (66)

[1] No carbocation is formed because it is not SN_1 reaction (49)

[1] $NaSCH_3$, DMSO are the intermediates to this reaction (10)

[1] An intermediate might be  **(16)**

[11] Identification of Nucleophiles/Electrophiles

[1] The SCH_3^- is the nucleophile. (35)

[1] Na^+ is the electrophile. (35)

[3] Br is acting as the nucleophile (28, 47, 48)

[1] Br underwent nucleophilic attack (10)

[1] Na^+ is a nucleophile looking for Br^- (49)

[3] SCH_3 is acting as the electrophile (28, 48, 70)

[1] $NaSCH_3$ is the electrophile (50)

[12] Types of Bonds

[2] Both molecules have 3 double bonds (34, 41)

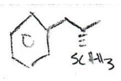
[1] This structure contains three double bonds (pi bond) (39) 

[1] There are 3 pi bonds in the substrate molecule (14)

[2] There is 6 sp^2 hybridized carbons in each molecule (5, 34)

[1] The reactants contains 6 sp^2 hybridized carbons. (35)

[1] 



and have a total of 12 sp^2 hybridized carbons (20)

[1] There are 6 double bonds in the benzene ring (4)

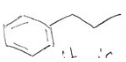
[1] Double bond contains one sigma and pi bond (39)

[1] Each benzene ring is sp^2 hybridized for each p orbital (67)

[1] The double bonds in the cyclohexene tells us that the molecule contains sp2 hybridization (17)

[20] Description of Bonding (Breaking/Forming)

[2] This is a one step reaction (48, 66)

[1] SCH_3 bonds to  *the same time Br leaves so it is into the page (9)*

[1] It is a one step reaction with Br leaving and SCH_3 coming at the same time (49)

[1] The DMSO helps remove the Br (72)

[1] Br attacks Na (47)

[2] This is a two step reaction (71, 79)

[1] Metal (Na) is used to remove Br from reactant (65)

[1] Na and DMSO will remove the bromine molecule (56)

[1] Na^+ bonds with Br^- to take it off the carbon. (35)

[1] Na breaks off Br from the molecule to form NaBr (22)

[1] Na reacts with Br to remove it from its position on the 2 carbon (16)

[1] The sodium is what takes the bromine away (61)

[1] Na from $NaSCH_3$ knocks off the Br. (4)

[1] After Na knocks off Br, SCH_3 is added in its place (4)

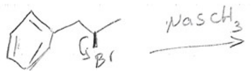
[1] During the reaction the Na^+ from $NaSCH_3$ will take Br off and replace with SCH_3 (29)

[1] When the Br leaves, there is a carbocation for the $^-SCH_3$ to bond to (13)

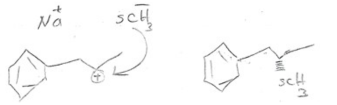
[1] A hydrogen anti to the bromine is removed (8)

[1] Na^+ masks the negative charge (48)

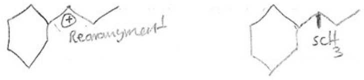
[3] Mechanism

[1] 

(73)

[1] 

(73)

[1] 

(73)

[21] Identification of Leaving Groups

[9] The bromine is acting as a leaving group (10, 12, 14, 25, 43, 49, 52, 61, 75)

[6] Br served as a good leaving group (3, 8, 56, 57, 64, 70)

[1] Br is a good leaving weak group (66)

[1] Br is a good leaving group, which allows for the SCH_3 to be substituted (1)

[1] The leaving group is tertiary (12)

[1] SCH_3 attacks Br because Br is a good leaving group (64)

[1] The leaving group is NaBr (76)

[1] Bromine is one of the best leaving groups (61)

[10] Identification of by-products

[8] A byproduct is NaBr (8, 9, 14, 22, 25, 32, 54, 70)

[1] During the reaction Br splits from the molecule and forms an ionic bond with Na (31)

[1] The Br bonds to the Na after leaving (15)

[17] Aromaticity

[3] Both of these molecules are aromatic (30, 62, 70)

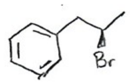
[4] Both molecules contain an aromatic ring (2, 53, 60, 76)

[2] Both product and reactant have an aromatic benzene ring (29, 55)

[1] The ring is aromatic (15)

[2] The benzene rings are aromatic (46, 71)

[1] Aromatic ring is unsaturated hydrocarbons. (39)

[1]  *is aromatic (57)*

[1] Neither compound is aromatic (8)

[1] Each benzene ring follows the equation 4n + 2 for number of electrons it contains (67)

[1] Aromatic (43)

[2] Resonance Structures

[1] Both have multiple resonance forms (53)

[1] The ring has resonance (54)

[10] Stability

[1] The result is more stable (69)

[1] The molecule on the right is the most stable (2)

[2] The product is more stable than the reactants (30, 50)

[1] The molecule becomes more stable after the reaction (46)

[1] –SCH_3 is more reactive than –Br (55)

[1] The rings shown are likely in chair formations, which are more stable than boat formations (57)

[1] It is a more stable molecule than any alkane (36)

[1] The product is less stable than the starting molecule (28)

[1] Both are relatively stable (53)

[5] Reaction Rate

[1] DMSO is a good solvent for SN_2 reactions (faster rate) (51)

[1] $NaSCH_3$ is a proton withdrawing group, and would make for a faster reaction time (1)

[1] This reaction will be slower than a normal benzene ring (63)

[1] The time it would take to react decreased (33)

[1] CH3 and OH react faster than benzene in electrophilic substitution reaction. (39)

[1] Directing Groups

[1] –Br is a weak deactivating group (63)

[17] Properties

[1] $NaSCH_3$ and **DMSO are** *reagents* **(74)**

[1] A aprotic solvent is used to help the reaction proceed (9)

[1] DMSO is an aprotic, and typically used for SN_2 reactions. (1)

[5] DMSO is a catalyst. (2, 6, 19, 27, 54)

[1] DMSO acts as a catalyst to speed up the reaction (17)

[1] The product is an acid (18)

[1] The one of the left is more acidic (53)

[1] DMSO is a common catalyst in benzene reactions (18)

[1] DMSO is a constitutional isomer (40)

[1] DMSO is acting as an enzyme (47)

[1] Catalyst – $NaSCH_3$ DMSO (43)

[1] The solvents is protic (12)

[1] Nucleotide – SCH_3 (43)

[27] Stereochemistry

[1] It is a chiral molecule (67)

[1] There is an inversion of configuration (49)

[1] It has one chiral carbon (63)

[4] One stereogenic carbon on each molecule in product and reactant (2, 52, 67, 78)

[1] One stereogenic carbon (19)

[1] Product contains a stereogenic carbon (11)

[2] The reaction takes place on a stereogenic carbon (25, 50)

[1] An inversion happened (66)

[1] Orientation of substituent group reverses (75)

[1] The orientation of the functional group is changed between the products and reactants (36)

[1] The product side, SCH_3 is in the down position which is drawn with  *(84)*

[2] The Br is pointing off the paper towards us (55, 79)

[1] Br and SCH_3 differ within 3-dimensionality within the molecule (10)

[2] Br is coming towards us while SCH_3 is going away. (6, 52)

[1] Br is coming out toward you (81)

[1] When this reaction happens, it goes from Br towards you to SCH_3 away from you (22)

[2] The SCH_3 is facing from us on the stereogenic carbon (55, 79)

[1] SCH_3 is going behind or away from you (81)

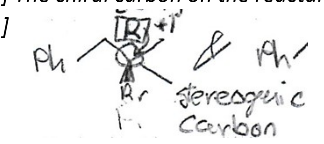
[1] The reactant side, Br is in the up position which is drawn with  ***(84)***

[1] Has stereochemistry (7)

[50] Configuration

[16] In the first molecule the Br is in the R configuration. (1, 5, 13, 17, 18, 19, 27, 30, 33, 38, ***40****, 45, 62, 63, 71, 76)*

[1] The chiral carbon on the reactant is R (31)

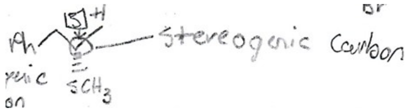
[1]  *(50)*

[1] The solution is a R configuration (15)

[1] The stereogenic carbon on the reactant side is right-handed (57)

[14] In the second molecule the SCH_3 is in the S configuration (1, 5, 11, 13, 17, 19, 27, 30, 33, 38, 45, 62, 63, 76)

[1] The chiral carbon on the product is S (31)

[1]  *(50)*

[1] The stereogenic carbon on the product side is left-handed (57)

[5] The SCH_3 is R-configuration (18, 40, 71, 72, 84)

[2] The Br is S-configuration (72, 84)

[1] Compound begins as cis and ends up in trans (33)

[1] Br and SCH_3 are trans in relation to each other (65)

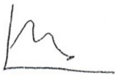
[1] -SCH_3 adds trans to the original –Br substituent (51)

[1] The two molecules are trans of each other since Br is in front and SCH_3 is in the back (17)

[1] The SCH_3 attached anti to Br (54)

[1] S configuration. (67)

[1] Reaction Energy Diagrams

[1] The graph would look like  **(58)**

[11] Miscellanea

[1] The reaction forces the Br and SCH_3 to flip resonance structures (46)

[1] This reaction cannot go in reverse because the bromine is too weak (46)

[1] DMSO is used to make the leaving group better (20)

[1] $NaSCH_3$ is a bulky base. That's why DMSO is needed to make the reaction start (51)

[1] The benzene ring makes it easier for a reaction to take place because of its aromaticity (12)

[1] If you cross out Na and make SCH_3 negative you can put it where Br is if its positive (84)

[1] DMSO caused Br to face away, go from wedge to dash (3)

[1] SN_2 reactions prefer polar protic solvents such as $NaSCH_3$ (20)

[1] This is an easily reversible reaction (69)

[1] Br wants to gain an electron. (6)

[1] This changes the structure and composition (6)