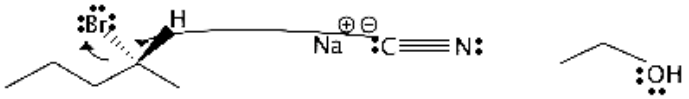
# APPENDIX A: PICTORIAL INSCRIPTIONS, AND VERBAL TRANSCRIPTIONS AND TRANSLATIONS

1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R) bromopentane ($C_5H_{11}Br$) reacts with sodium cyanide (NaCN) using ethanol as the solvent.

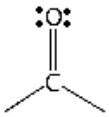



(R)-2-Bromopentane Sodium cyanide Ethanol

The Br leaves and the C on the cyanide throws its electrons at the C that Br left from for an $SN_2$ reaction.

Another thing that happens is an $E_2$ reaction where the Br leaves and the cyanide pulls an H off of the 3rd carbon in bromopentane, causing a double bond to form between carbons 2 and 3.

2. Explain why the #2 products of the reaction in #1 are formed faster if the solvent is switched to acetone.




Acetone

Because acetone is more polar and helps stabilize charges. This stabilization lowers the NRG that is required for the reaction to happen.

File:wk8S,MC

| Verbal Transcription | Translation/Interpretation |
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| At the top of the text, the first verbal part of the quiz question and the accompanying labeled molecular drawings of (R)-2-bromopentane, sodium cyanide, and ethanol are shown. | |
| The student has altered the drawing of 2-bromopentane and sodium cyanide by drawing a curved arrow from the two dots to the left of the "C" to the 4th vertex (L to R) of the 2-bromopentant. There is an additional arrow curving upwards from that vertex to the "Br" | The student does not redraw the molecules, nor does the student rearrange them into a more conventional chemical equation format. The student does not draw the products of the reaction. The student shows the $S_N2$ reaction of the cyanide ion with bromopentane with the bromine as a leaving group. Not redrawing the molecules could signify the student's lack of confidence in either 1) drawing the molecules correctly or 2) using the program correctly to draw the molecules. Or perhaps it is an ease of use issue. |

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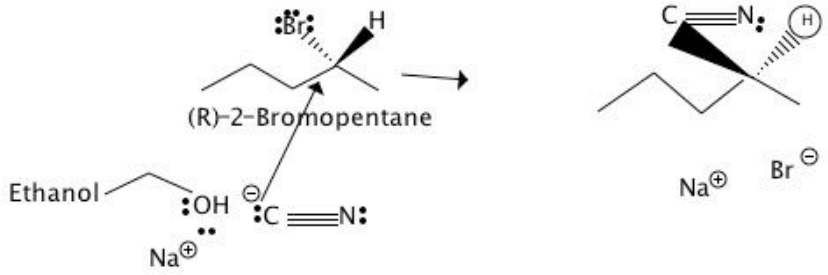
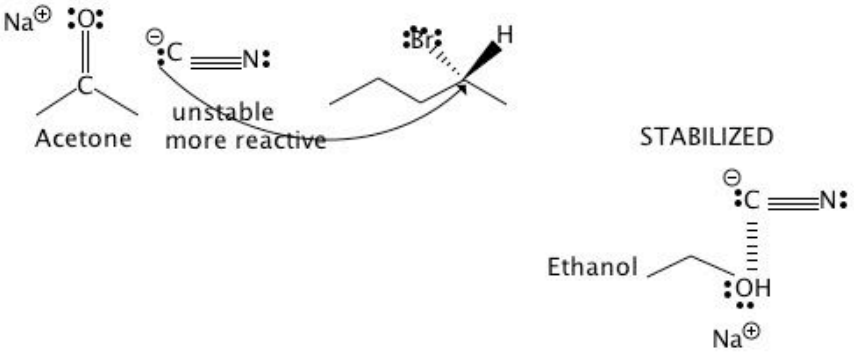
| The student has added the following text below the drawings: "The Br leaves and the C on the cyanide throws its electrons at the C that Br left from for an $S_N2$ reaction. Another thing that happens is an E2 reaction where the Br leaves and the cyanide pulls an H off the 3rd carbon in bromopentane causing a double bond to form between carbons 2 and 3. | The student explains the reaction in words. However, the wording implies a two step reaction:<br>1) the Br leaves,<br>2) *and* the C on the cyanide *throws* it's electrons at the C that Br *left* from for an $S_N2$ reaction (emphasis mine)<br>In the $S_N2$ reaction, bond making and bond breaking occur simultaneously. The apparent simultaneous reaction path implied by the drawing does not display, perhaps, the student's true understanding of the path of this reaction.<br><br>The student continues by discussing the possibility of an E2 reaction, which is not shown graphically.<br><br>By not drawing the products of the $S_N2$ reaction, nor the progress or products of the E2 reaction, the student ignores the issue of stereochemistry, prompted by the verbal stereochemical designation of the reactant, (R), and the pictorial drawing of stereochemistry using wedges and dashed lines. However, the student does recognize that inversion of configuration occurs based on the answer to the verbal quiz. |
| In the middle of the text, the second verbal part of the quiz question and the accompanying labeled molecular drawing of acetone is shown.<br><br>The student's answer is entirely verbal: "Because acetone is more polar and helps stabilize charges. This stabilization lowers the NRG that is required for the reaction to happen." | The student does not draw any charged species to illustrate the answer, nor does s/he specify which charged species are referred to. The only charged species shown is the sodium cyanate. However, partial charges do form on molecules during $S_N2$, and E2 reactions. Acetone is not more polar than ethanol, and would not stabilize these charges. Instead, ethanol competes with the reaction by participating itself. |

1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R)-2-bromopentane ($C_5H_{11}Br$) reacts with sodium cyanide (NaCN) using ethanol as the solvent.




2. Explain why the $S_N2$ products of the reaction in #1 are formed faster if the solvent is switched to acetone.




File: wk8Se,S

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The verbal portion of the first question is shown at the top of the text. | |
| Beneath the text is a labeled molecular drawing of (R)-2-bromopentane. To the right is a rightward facing arrow. To the right of the arrow is a molecular drawing of (S)-2-cyanopentane. Beneath the (S)-2-cyanopentane is Na with a plus sign slightly above and to the right, and Br with a minus sign slightly above and to the right. | The student shows an $S_N2$ reaction. The student draws the products of the reaction with inversion of configuration. |
| Below the (R)-2-bromopentane is drawn a labeled molecular drawing of ethanol. To the right of the ethanol drawing is a picture of cyanide with a minus sign slightly above and to the left of the C. There is an arrow pointing from the electron dots on the C | Given the drawing in the lower right of the text, the student appears to be drawing the interaction between the solvent, ethanol, the cyanide anion, and the sodium cation. |

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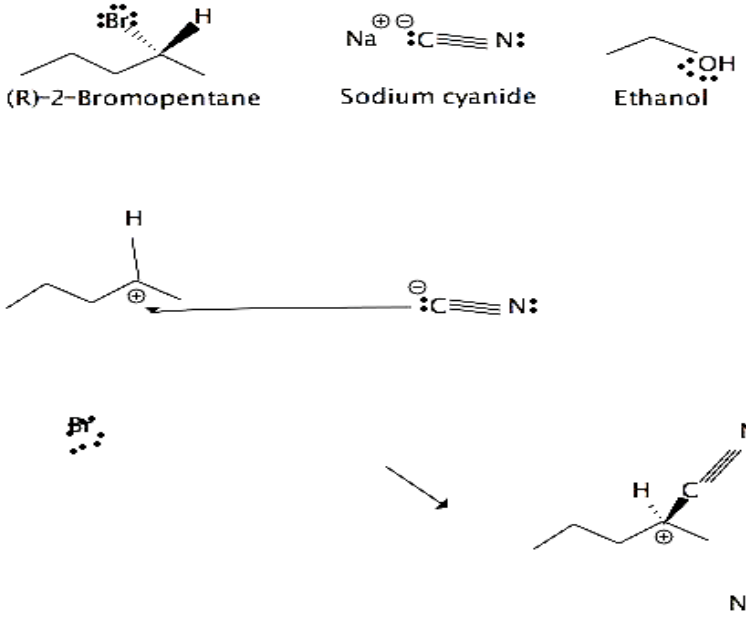
| toward the 2nd carbon of pentane. Below the O of ethanol is drawn an Na with a plus sign slightly above and to the right. | |
| The text of the second question is shown in he approximate middle of the text. | |
| Below the text of the second question is a labeled molecular drawing of acetone. To the left of the O of acetone is Na with a plus sign slightly above and to the right. To the right of the acetone drawing is a picture of the cyanide with a minus sign slightly above and to the left of the C. To the right of the cyanide is a molecular drawing of (R)-2-bromopentane. | The student appears to be drawing the interaction between acetone, the cyanide anion, and the sodium cation. This picture mirrors the drawings of the ethanol interaction above and below. |
| There is an arrow drawn from the dots on C of cyanide toward the 2nd carbon on the (R)-2-bromopentane. | The student redraws the $S_N2$ reaction in an attempt to explain the interaction between the solvent and the reaction mechanism. |
| The words "unstable more reactive" are written underneath the cyanide. | These words attempt to explain how the interaction drawn above influences the mechanism of the $S_N2$ reaction. |
| In the lower right corner of the text is a labeled molecular picture of ethanol. Above the ethanol O is a drawing of cyanide with a minus sign slightly above and to the right of the C. There is a dashed line between the C of the cyanide and the O of ethanol. Below the O is an Na with a plus sign slightly above and to the right of the Na. Above these drawings is the word "Stabilized". | This picture appears to be a drawing the interaction between ethanol, the cyanide anion, and the sodium cation. The word "stabilized" attempts to explain how this interaction does not favor the $S_N2$ reaction, though the mechanism of the reaction is not shown. |




$Sn_1$ is slower than $Sn_2$ because carbocations are a lot of energy
Acetone promotes $Sn_2$. Thus it is faster

File: wk8N,AT

| Verbal Transcription | Translation/Interpretation |
|---|---|
| At the top of the text, the three labeled molecular drawings of (R)-2-bromopentane, sodium cyanide and ethanol are shown. These are unaltered from the original depiction in the quiz question. | |
| On a "line" below the molecular drawings of the reactants, are two more molecular drawings. The drawing on the left is similar to (R)-2-bromopentane, but the Br is missing, along with the accompanying dark wedge and 6 dots. In addition, what was a the dashed wedge accompanying the H is now a simple line. There is a plus sign at the #2 carbon. | The student appears to be showing the loss of bromine in an earlier (not shown) step to form the carbocation and the Br drawn below it. The student has also drawn the loss of stereochemistry accompanying the formation of the carbocation. The formation of a carbocation in an initial step corresponds to an $S_N1$ reaction. |
| The drawing on the left is the cyanide portion of the sodium cyanide shown above along with a minus sign. This appears to be pasted from the line above. There is an | The negatively charged cyanide ion is attracted to the positively charged carbocation; the ewis base donates electrons to the Lewis acid. |

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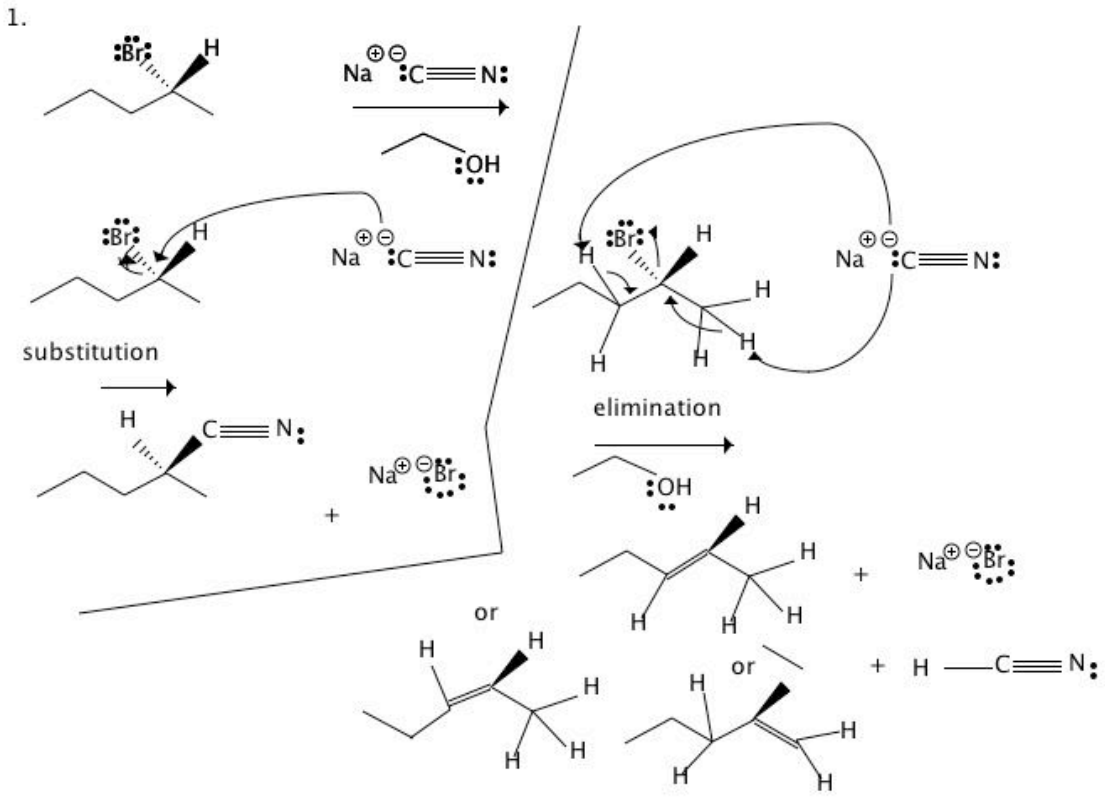
| arrow pointing to the left from the two dots next to C toward the plus sign. | |
| On a third "line" is a Br with 8 dots around it on the left. On the right is an arrow pointing from above and to the left, toward the lower left, in general, at two more molecular drawings.<br><br>The first is similar to the original drawing of R)-2-bromopentane, but the Br has been replaced by an H, and the H has been replaced by the cyanide. There is a plus sign at the #2 carbon. Down and to the left is written NaBr | This bromine appears to accompany the carbocation on the second line.<br><br>The products are formed. The student has correctly shown inversion of configuration, which would occur form an $S_N2$ reaction, but racemization would occur for an $S_N1$. The student has also balanced the equation by indicating the formation of sodium bromide. The plus sign could be a remnant of pasting the pentane from the previous line |
| Beneath, at the bottom of the text is written, "$S_N1$ is slower than $S_N2$ because carbocations are a lot of energy. Acetone promotes $S_N2$. Thus it is faster" | The student does not draw an answer to the second question, but explains that the formation of a carbocation (separation of charge) requires more energy. The student states that acetone promotes $S_N2$ reactions, but does not explain why. |




2. The acetone makes the reaction go faster because it doesn't have the polarity of the H and O bond and therefore doesn't interfere with the substitution reaction

File: wk8N‚J

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The answer to the first question is arranged in two sets of molecular diagrams separated by a line shaped like a backwards L. | The student has shown both the possibility of substitution and elimination. |
| In the grouping on the left, (R)-2-bromopentane is shown on the left side of a rightward facing arrow. Sodium cyanide is shown above the arrow, and ethanol is shown below. These pictures appear to be copied from the original pictures in the quiz question, based on the placement of bonds, charges, atom labels, and dots. | The student appears to copy-and-paste the overall skeleton of pentane throughout the text. This copy-and-pasting could signify the student's lack of confidence in either 1) drawing the molecules correctly or 2) using the program correctly to draw the molecules. Or perhaps it is an ease of use issue. |
| Below, (R)-2-bromopentane is redrawn along with sodium cyanide. A rightward facing curved arrow is drawn from the | The student shows an $S_N2$ reaction. The student's written verbal quiz response only refers to substitution, |

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| minus sign on the cyanide to the 2nd carbon on bromopentane. A small curved arrow points from the 2nd carbon upward to the bromine. The word "substitution" is written underneath the pentane. There is a small rightward facing arrow under the word "substitution" | |
| Under the rightward facing arrow is a picture of (S)-2-cyanopentane. To the left is a plus sign and the formula NaBr. There is a plus sign to the upper right of the Na, and a minus sign to the upper left of the Br. In addition, 4 pairs of dots are clustered around the Br. | The student includes inversion of configuration in the drawing. Inversion of configuration is also discussed in the written verbal quiz. |
| In the right grouping of diagrams, (R)-2-bromopentane and sodium cyanide are copied again. The pentane has been modified by drawing bonds to H on carbon 1 and 3. There are several arrows drawn between and around these diagrams. One curved arrow proceeds from the two dots on sodium cyanide downward and to the left to point at an H on carbon 1. There is a curved arrow pointing to the left from the bond between that H and the C to the 2nd carbon. There is another arrow curving upward and to the left from the minus sign on the cyanide toward an H drawn on the 3rd carbon. Another arrow proceeds downward from that H to the bond between carbons 2 and 3. One final arrow curves from the second carbon to the bromine on carbon 2. | The student also shows E2 elimination. There are two possibilities: elimination of a primary hydrogen atom at carbon #1, or elimination of a secondary hydrogen atom at carbon #3. The student shows both possibilities in one set of diagrams. |
| Under the pentane diagram is the word "elimination." Under that is a rightward facing arrow, and under the arrow is a molecular diagram of ethanol. | |
| Under the diagram of ethanol are 3 molecular diagrams. The first is *trans*-2-pentene. Under that and to the left is *cis*-2-pentene, and to the right is 1-pentene. The student retains the wedge shaped bond to | The student shows all possible elimination products. The incorrect retention of the wedge shaped bond to hydrogen on carbon #2 maybe a result of copy-and-pasting from the previous drawings. |

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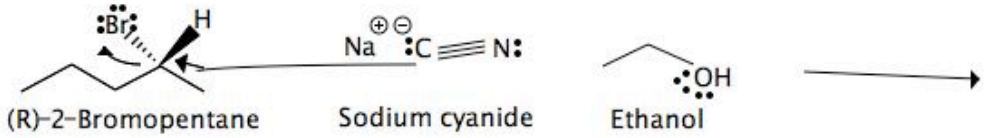
| an H on the 2nd carbon in all product diagrams. | |
| To the left of these diagrams are two more diagrams. Above, is a molecular formula NaBr. There is a plus sign to the upper right of the Na, and a minus sign to the upper left of the Br. In addition, 4 pairs of dots are clustered around the Br. This diagram appears to be copied from the other one, based on the position of the dots and charges, and the relationship between the Na and Br symbols.<br><br>Below, is a structural formula of hydrocyanic acid. | The two additional products are correctly shown. |
| Written below all this is: "2. The acetone makes the reaction go faster because it doesn't have the polarity of the H and O bond and therefore doesn't interfere with the substitution reaction." | The student offers a significantly more detailed answer in the written verbal quiz: "Ethanol adds the possibility of hydrogen bonding to the system through the hydroxide group. The (R)-2-bromopentane and the cyanide participate in hydrogen bonding with the ethanol which makes the reaction in 1. Less likely to happen. When the solvent is acetone, this stabilizing hydrogen-bonding does not occur, making the reaction more likely to happen. Hydrogen-bonding doesn't get in the way and keep the reactants from interacting with one another. The same reaction occurs, but it occurs faster." It is unclear why the student answers in so much more detail on the written verbal quiz than on the pictorial quiz. |

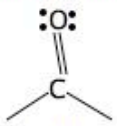
1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R)-2-bromopentane ($C_5H_{11}Br$) reacts with sodium cyanide (NaCN) using ethanol as the solvent.



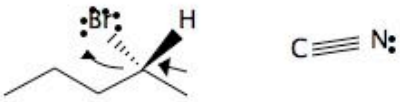

(R)-2-Bromopentane  Sodium cyanide  Ethanol


( s) – 2⁻ cyanopentane

2. Explain why the $S_n2$ products of the reaction in $\#_1$ are formed faster if the solvent is switched to acetone.




Acetone




File: wk8N‚JM

| Verbal Transcription | Translation/Interpretation |
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| At the top of the text, the quiz question is retained, and the three labeled molecular drawings of (R)-2-bromopentane, sodium cyanide and ethanol are shown. | Not redrawing the molecules could signify the student's lack of confidence in either 1) drawing the molecules correctly or 2) using the program correctly to draw the molecules. Or perhaps it is an ease of use issue. |
| The student alters the labeled molecular drawings by drawing a leftward facing curved arrow from the cyanide carbon to the 2nd carbon on (R)-2-bromopentane. There is another arrow curving upward from the 2nd carbon towards the Br. A rightward facing arrow is draw to the right of these drawings. | The student shows an $S_N2$ reaction. |
| On the next "line" below the first drawings, is drawn a molecule labeled "(s)-2-cyanopentane" in which the cyanide group | The products of the $S_N2$ reaction are shown with inversion of configuration. |

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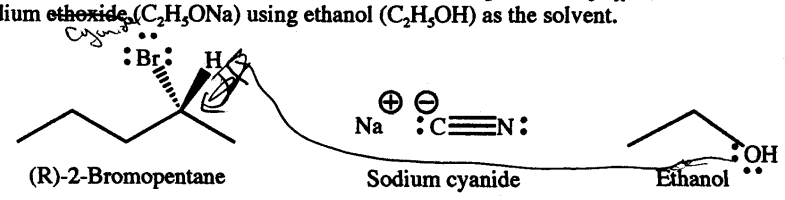
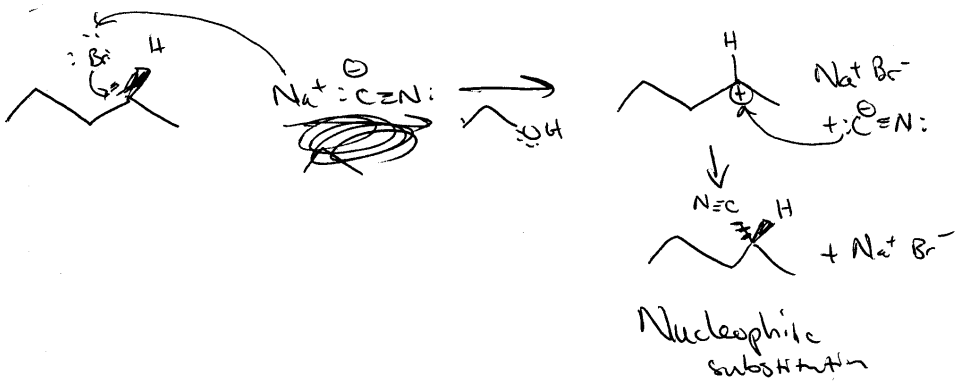
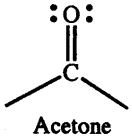
| is attached to the second carbon via a wedge, and the hydrogen is now attached using a dashed line. To the right is the formula NaBr. Above the Na is a plus sign. Above and to the right of the Br is a minus sign. To the right, is ethanol, unchanged from the picture above. | |
| The second question is shown below these drawings, along with the unchanged drawing of acetone. There are additional pictures of (R)-2-bromopentane and cyanide. The pentane is shown with two small arrows, one pointing at the 2nd carbon, and one pointing upward from the second carbon toward the Br. The cyanide has been modified by removing the electron dots and the minus sign on the C. | The student does not answer the second question. The drawings shown here appear to be the same as pieces of the drawings above. Perhaps this was the beginning of an answer to the question which the student did not finish. |

**1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R)-2-bromopentane ($C_5H_{11}Br$) reacts with sodium ~~ethoxide~~ ($C_2H_5ONa$) using ethanol ($C_2H_5OH$) as the solvent.**

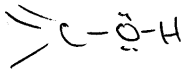



**2. Explain why the $S_n^2$ products of the reaction in #1 are formed faster if the solvent is switched to acetone.**




Acetone is more likely to take off the hydrogen in the C-H location since it stabilizes itself through resonance. By taking the H off ~~sooo~~ quicker the cation is formed and the reaction proceeds.



File: wk8AP,KZ

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The student has altered the drawings given in the quiz question, and provided other drawings in the space below. The student has drawn an arrow from the lone pair of electrons on ethanol to the area of the hydrogen on (R)-2-bromopentane. However, the student has crossed out the | Given the way that the arrow is drawn, it isn't possible to discern the student's intent with the first arrow. |

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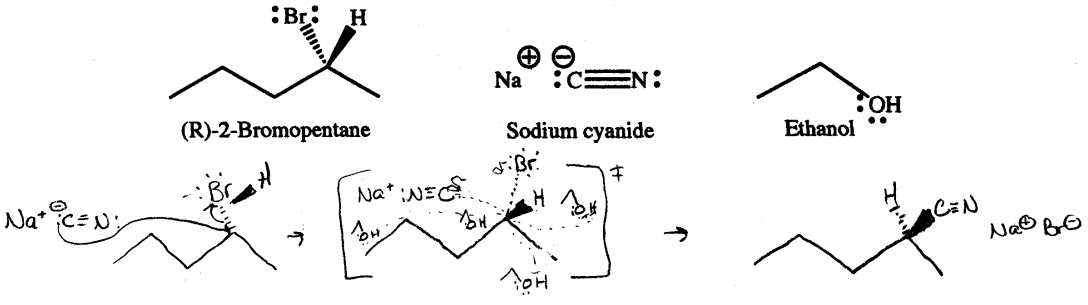
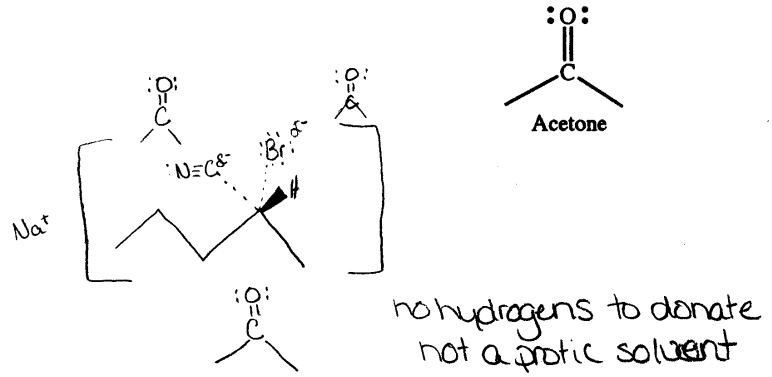
| arrowhead end of the arrow. | |
| In the space below the quiz, the student has redrawn (R)-2-bromopentane and sodium cyanide, including the appropriate charges. An arrow is drawn from the Na of sodium cyanide pointing toward the Br. Another arrow is drawn from the Br to C#2. | The student appears to be showing a reaction between the sodium and the bromide but does not properly account for electrons. |
| To the right of the cyanide is drawn a right-pointing arrow, underneath which is a drawing of ethanol. To the right of this arrow is a pentane molecule which is missing the Br, has a + at C#2, and the H is connected with a line rather than a wedge. To the right of the pentane picture and above the CN is drawn NaBr with the appropriate charges. | The student has drawn a carbocation at C#2, and shown NaBr, apparently as a product. |
| The student redraws the cyanide ion with an arrow pointing toward the + on C#2 | The student is showing a reaction between the negatively charged CN and the positively charged C#2. |
| The student draws an arrow downward from the carbocation pointing toward a picture of (R)-2-cyanopentane. NaBr with charges is drawn to the right of the pentane molecule, a "+" is placed between them. Below these pictures is a label: "Nucleophilic substitution" | The student shows retention of configuration. |

1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R)-2-bromopentane ($C_5H_{11}Br$) reacts with sodium ethoxide ($C_2H_5ONa$) using ethanol ($C_2H_5OH$) as the solvent.




2. Explain why the $S_n^2$ products of the reaction in #1 are formed faster if the solvent is switched to acetone.




File wk8CM,EF

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The student has redrawn (R)-2-bromopentane underneath the original drawing on the left side of the page. The depiction is slightly altered with the wedge and H symbol being placed so that it looks like it is coming from the Br, rather than the original location | This is likely just a mistake, as the student does not continue it through the rest of the problem, nor does the student make the same mistake in part 2 of the problem. |
| To the left of the bromopentane drawing, the student has drawn sodium cyanide, in the same way it was presented in the quiz question. There is a curved arrow leading from the lone pair of the C in cyanide to | The student is showing the traditional curved arrow depiction of an $S_N2$ reaction showing the cyanide ion attacking carbon #2, and the bromine is the leaving group |

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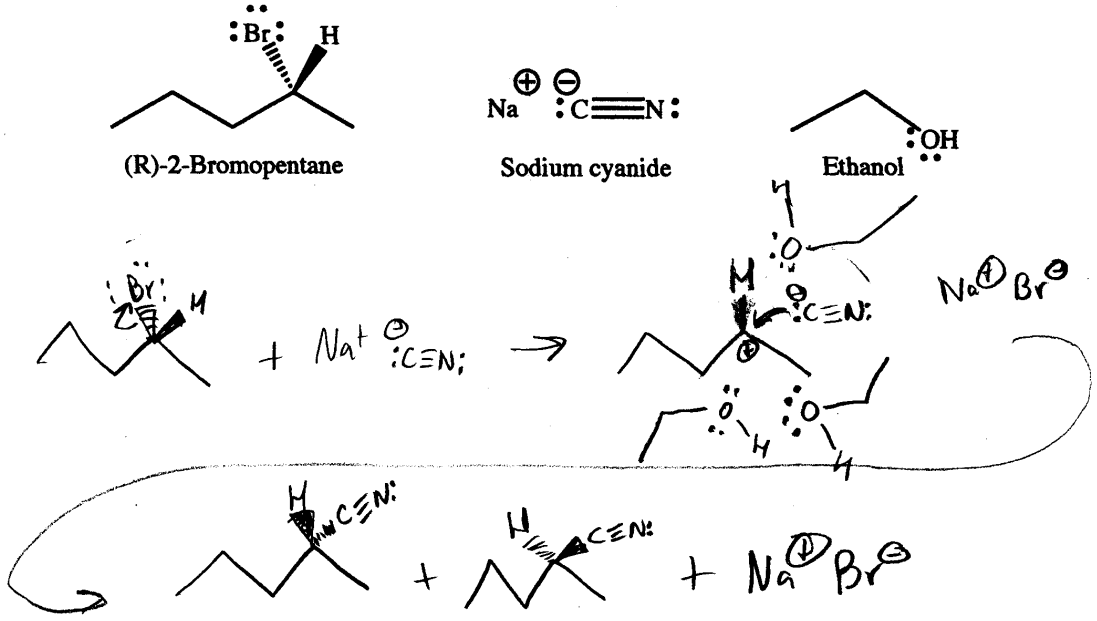
| carbon #2 of the bromopentane. There is another arrow drawn from carbon #2 to the bromine. | |
| To the right of these drawings there is an arrow pointing to a group of drawings inside brackets. The rightmost bracket has a double-dagger superscript. | The student has show the transition state of an $S_N2$ reaction |
| Inside the brackets, the bromopentane is redrawn, however, the Br is now attached using a dotted line rather than a dashed wedge. There is also a dotted line coming from the C in cyanide (which has now been turned around to face carbon #2. A partial negative symbol ($\delta^-$) is placed next to the Br and next to the C of cyanide. Small depictions of ethanol are drawn around the bromopentane molecule with small dotted lines drawn between the ethanol and bromopentane. | The student has shown the transition state with the forming C-C bond and the breaking C-Br bond. However the student has not accounted for the inversion of configuration of the stereochemistry in this drawing as carbon #2 is not planar. The H is still drawn with a wedge.<br><br>The student has attempted to depict solvation by ethanol. The ethanol molecules are drawn considerably smaller than the bromopentane. It is not clear if the student believes that ethanol is really that much smaller than the bromopentane or if the student is just forgrounding the changes going on with the reactants and making the solvation less salient. |
| To the right of the brackets is another right-pointing arrow. To the right of this arrow is a depiction of (S)-2-cyanopentane. To the right of the (S)-2-cyanopentane is a drawing of sodium bromide using elemental symbols and charges. | The student has properly drawn the results of an $S_N2$ reaction. |

**1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R)-2-bromopentane ($C_5H_{11}Br$) reacts with sodium ethoxide ($C_2H_5ONa$) using ethanol ($C_2H_5OH$) as the solvent.**




File wk8CM,MP

| Verbal Transcription | Translation/Interpretation |
|---|---|
| On the left side of the paper, the student has redrawn (R)-2-bromopentane. There is a curved arrow pointing upward from the bond between the Br and C#2 toward the Br. | The student appears to be indicating that the bromine leaves the pentane molecule |
| To the right of the drawing of bromopentane is a "+" sign and sodium cyanide is redrawn with the charges indicated. To the right of this is a rightward pointing arrow. | |
| To the right of the arrow the student has drawn a pentane molecule. The Br is gone, and the H is now bonded with a line instead of a dashed wedge. There is a "+" at C#2. The molecule has several drawings of ethanol around it, pointed so that the lone pair electrons are arranged near C#2. There is a cyanide ion drawn and an arrow is pointing from the lone pair on the cyanide C to C#2. To the right of these drawings, NaBr, with appropriate charges is drawn. | The student is indicating an $S_N1$ reaction in which the bromine leaves (previous step) and the cyanide acts as a nucleophile. |

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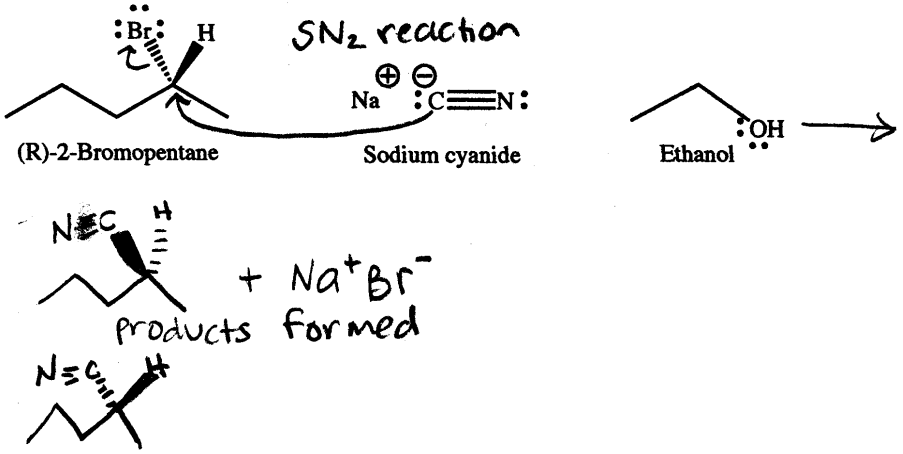
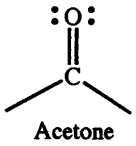
| There is a large arrow that points to the beginning (the left) of the next line. | Indicating products. |
| 3 drawings on this line, from left to right: (R)-2-cyanopentane, (S)-cyanopentane, and NaBr are drawn. | The student draws products for the retention and inversion of configuration. |

1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R)-2-bromopentane ($C_5H_{11}Br$) reacts with sodium ethoxide ($C_2H_5ONa$) using ethanol ($C_2H_5OH$) as the solvent.




2. Explain why the $S_n^2$ products of the reaction in #1 are formed faster if the solvent is switched to acetone.




ethanol is a more polar solvent, acetone doesn't "split up" the the sodium cyanide as much and if the sodium cyanide has 2 ions with distinct charges, it is more likely to react with the (R)-2-Bromopentane.

File: wk8DB,ES

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The student has modified the structural drawings printed with the quiz question. The student has drawn an arrow from the C on the cyanide ion to C#2 on the bromopentane structure. There is an additional arrow drawn from C#2 to the bromine. There is a label above the cyanide, "$S_N2$ reaction." To the right of the | The student has drawn the traditional curved arrows indicating an $S_N2$ reaction between cyanide ions as the nucleophile and the bromopentane, with Br as the leaving group |

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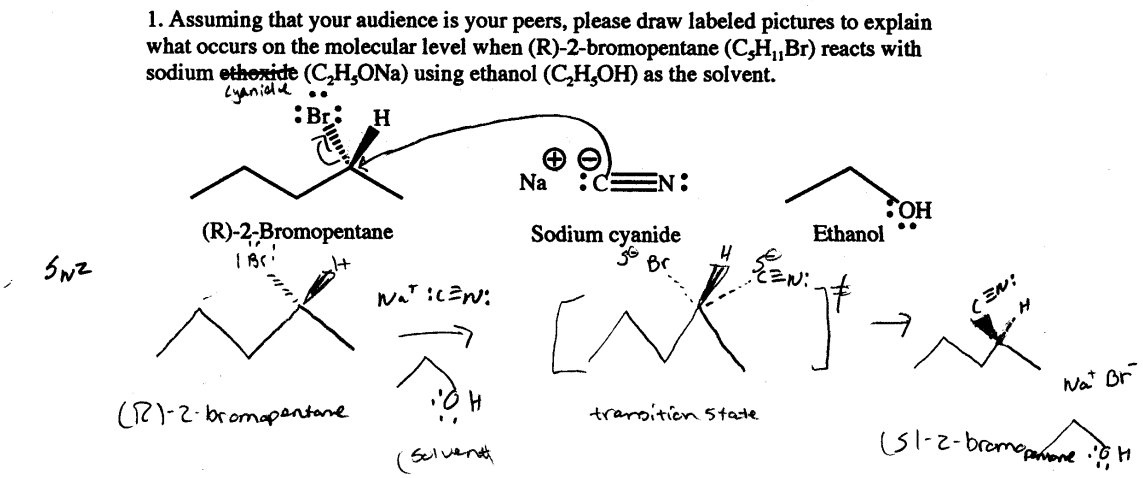
| drawing of ethanol is a right pointing arrow. | |
| In the space provided, below the drawings of bromopentane, sodium cyanide, and ethanol, the student has drawn 3 structures. The first is a structure of (S)-2-cyanopentane. To the right of this structure, separated by a "+" sign is drawn NaBr with charges included. Below these drawings is written, "products formed." Below that label is drawn a picture of (R)-2-cyanopentane. | The student has drawn the products, but included the product resulting form retention of configuration, which does not happen in an $S_N2$ reaction as labeled. |




File wk8DB,KK

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The student has modified the drawings already present in the printed quiz question. In addition, the student has written several structures below the quiz question in the space provided | The student appears to have shown the general curved arrow mechanism of an $S_N2$ reaction on the quiz question itself, then provided more details below that. |
| Using the structures provided in the quiz question, the student has drawn a curved arrow from the C of CN to carbon #2 on (R)-2-bromopentane. The student has drawn another curved arrow from carbon #2 to the bromine | The student has drawn the traditional curved arrow mechanism for an $S_N2$ reaction with the cyanide ion as the nucleophile attacking C#2 and Br as the leaving group |
| In a "line" below the structures drawn for the quiz question, the student has, on the left side, redrawn (R)-2-bromopentane and labeled it as such. To the right of this structure, is a right pointing arrow over which is drawn the structure for sodium cyanide. Under the arrow is drawn the structure for ethanol which is labeled with the word "(solvent)" | The student is showing the reactants in the traditional fashion |
| To the right of the arrow is a structure drawn inside brackets. The right bracket has a "double-dagger" superscript. Inside the brackets, the bromopentane is redrawn, however, the Br is now attached using a | The student has shown the transition state with the forming C-C bond and the breaking C-Br bond. However the student has not accounted for the inversion of configuration of the stereochemistry in this |

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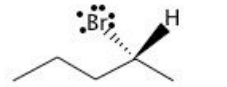
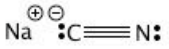
| dotted line rather than a dashed wedge. There is also a dotted line coming from the C in cyanide (which has now been turned around to face carbon #2. A partial negative symbol ($\delta^-$) is placed next to the Br and next to the C of cyanide. This drawing is labeled "transition state." | drawing as carbon #2 is not planar. The H is still drawn with a wedge. |
| To the right of the brackets is a right pointing arrow and the structure of (S)-2-cyanopentane is drawn along with a structure of NaBr including charges, and the name (s)-2-bromopentane is written. The structure of ethanol is redrawn. | The student has drawn one of the possible products of this reaction along with the remaining spectator ions. The name (S)-2-bromopentane does not appear to be a label for the drawing of the cyanopentane, but instead seems to indicate another possible product. |

ADVANCED GROUP

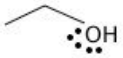
1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R)-2-bromopentane ($C_5H_{11}Br$) reacts with sodium cyanide (NaCN) using ethanol as the solvent.



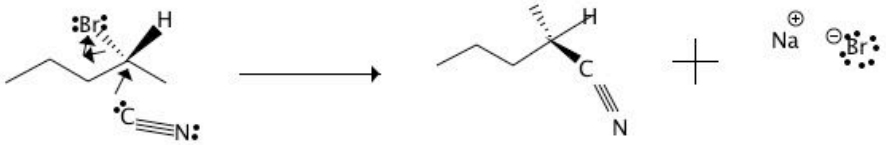
(R)-2-Bromopentane



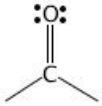
Sodium cyanide



Ethanol



2. Explain why the $S_n2$ products of the reaction in #1 are formed faster if the solvent is switched to acetone.



Acetone

This reaction, which slows down the overall reaction, does not occur if acetone is used

file: wk8AdvSR

| Verbal Transcription | Translation/Interpretation |
|---|---|
| In the space below the quiz, it appears that the student has redrawn (R)-2-bromopentane, or modified the original drawing by removing one set of electrons from the bromine atom. However, the student may have simply recopied the molecular drawing and missed one set of electrons. Underneath the (R)-2-bromopentane, the student has drawn a cyanide ion, without a negative charge. An arrow is pointing upward from the electron pair on the carbon atom of cyanide towards the second carbon. Two additional arrows are drawn from the bond between the 2nd carbon and the bromine atom pointing toward the bromine atom. | The student shows an $S_N2$ reaction. |

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|---|---|
| To the right of these drawings is a right facing arrow. | |
| To the right of the arrow is a structure drawn which looks like a modified version of (R) bromopentane. However, the cyanide group is now attached at the 2nd carbon. Carbon one is now shown to be pointing into the plane of the paper using the dashed wedge convention, the hydrogen is in the plane of the paper using a solid bond, and the cyanide group is shown pointing out of the plane of the paper using a dark wedge. The stereochemistry of the 2nd carbon is not specified because the drawing is non-standard: the dashed bond and dark wedge are on opposite sides of the in-plane bonds. To the right of this structure is a large plus sign. | The student shows a product of an $S_N2$ reaction but the stereochemistry is ambiguous because the drawing does not follow typical drawing conventions. |
| An Na with a plus sign is shown to the left of a Br symbol with 8 dots and a negative sign. | Sodium bromide is another product of the reaction |
| Below question 2, the student has drawn the structure of ethanol. Using a structural drawing which omits atom labels except for the O and H of the alcohol group. To the right of this structure, the student has copied the cyanide ion from the quiz question. An arrow is drawn from the electron pair on the cyanide carbon toward the H of the alcohol group. Two additional arrows are shown pointing from the bond between O and H, toward the O | The student shows deprotonation of alcohol by cyanide ions. |
| To the right of these structures is a right facing arrow | |
| Above and slightly to the right of the arrow is a copy of the ethanol structure. However, 6 electron dots have been added, the bond between the O and H, as well as the H, have been deleted, and a negative charge has been added. To the right of this | The student draws the products of a deprotonation of ethanol by sodium cyanide: sodium ethoxide and hydrocyanic acid.<br><br>The student writes, "This reaction, which |

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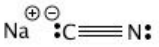
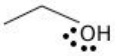
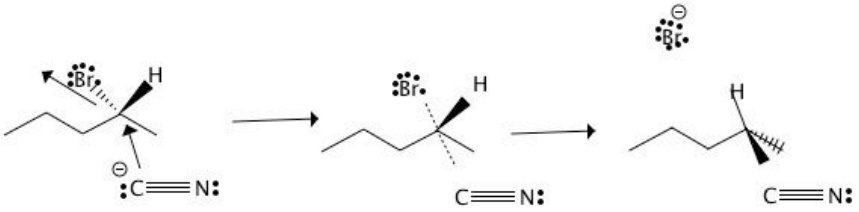
| structure is an Na with a positive charge. Below and to the right of this structure is the cyanide ion however, the electron pair on the carbon has been deleted as has the negative charge. Instead a bond is drawn from the carbon to an H. | slows down the overall reaction, does not occur if acetone is used. |
| The acetone structure drawn on the quiz has been moved to the right, out of the way of the answer. | |

1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R)-2-bromopentane ($C_5H_{11}Br$) reacts with sodium cyanide (NaCN) using ethanol as the solvent.

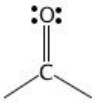

(R)-2-Bromopentane


Sodium cyanide

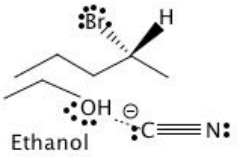

Ethanol



2. Explain why the $S_n^2$ products of the reaction in #1 are formed faster if the solvent is switched to acetone.


Acetone

Acetone will not block the reactants from interacting with each other


Ethanol

file: wk8AdvWG

| Verbal Transcription | Translation/Interpretation |
|---|---|
| In the space below the quiz, it appears that the student has copied the original drawing of (R)-2-bromopentane. Underneath the (R)-2-bromopentane, it appears that the student has copied the cyanide ion. An arrow is pointing upward from the electron pair on the carbon atom of cyanide towards the second carbon. An additional arrow is drawn from the bond between the 2nd carbon and the bromine atom pointing past the bromine atom. | The student shows an $S_N2$ reaction. |
| To the right of these drawings is a right facing arrow. | |
| To the right of the arrow is a copy of the (R)-2-bromopentane with several changes. The dashed wedge between the 2nd carbon and the bromine has become a dotted line. Another dotted line is drawn between the 2nd carbon of the pentane and the carbon of the cyanide. | The $S_N2$ transition state is shown. |

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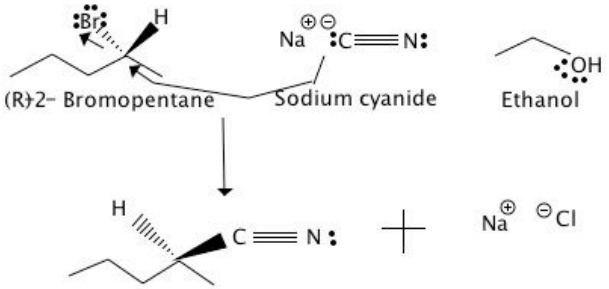
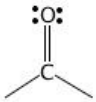
| To the right of these drawings is a right facing arrow. | |
| The pentane structure is recopied with changes. The bromine is now gone and there is a bold wedge between the 2nd carbon and the cyanide carbon atom. The hydrogen is now moved upwards and is drawn with a solid line. The bond to the carbon atom is overlaid with a dashed wedge. Above this structure is a Br with 8 dots and a negative charge. | The student has drawn (S)-2-cyanopentane as a product along with the bromide ion. |
| Underneath the second question the (R)-2-bromopentane is copied. Below that drawing, the structure of ethanol is copied with its label, and the picture of the cyanide ion with its negative charge and electrons. A dotted line is drawn between the carbon of the cyanide and the hydrogen of the ethanol. | The student writes, "Acetone will not block the reactants from interacting with each other." It appears that the student is drawing an interaction between the cyanide ion and the ethanol, which interferes with the interaction between the cyanide ion and (R)-2-bromopentane. |

1. Assuming that your audience is your peers, please draw labeled pictures to explain what occurs on the molecular level when (R)-2-bromopentane ($C_5H_{11}Br$) reacts with sodium cyanide (NaCN) using ethanol as the solvent.

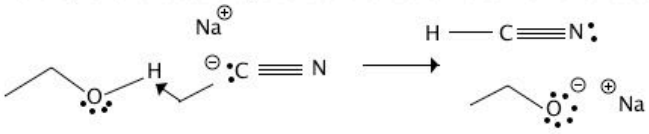



2. Explain why the $S_n2$ products of the reaction in #1 are formed faster if the solvent is switched to acetone.




Acetone won't react with any of the reactants, but ethanol could react with the reactants.

For Example



file: wk8AdvYX

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The student modifies the drawings on the quiz question by drawing an arrow from the cyanide carbon to the 2nd carbon of (R)-2-bromopentane. Another arrow is drawn from the bond between the 2nd carbon and the bromine of (R)-2-bromopentane pointing past the bromine. | The student shows an $S_N2$ reaction. |
| A downward pointing arrow points from the between the (R)-2-bromopentane and the sodium cyanide. | |
| Below the arrow, the student has drawn (S)-2-cyanopentane. To the right of the (S)-2-cyanopentane is a large plus sign. To the right of the plus sign is an Na with a positive charge, and to the right of that, a Cl with a negative charge. | The student shows the products of the $S_N2$ reaction as (S)-2-cyanopentane and sodium chloride. The student writes, "Acetone won't react with any of the reactants, but ethanol could react with the reactants. For Example" |
| Underneath the second question the student has drawn ethanol structure including the bond between the hydrogen and the oxygen | The student shows the deprotonated of ethanol by the cyanide ion |

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| (which are labeled) and included 4 dots around the oxygen. To the right of this drawing is the cyanide ion, with a negative charge on the carbon and two dots. However, the dots are missing from the nitrogen. An arrow is drawn from the cyanide carbon to the H on the ethanol OH. Above the cyanide is an Na with a positive charge. | |
| To the right of these drawings is a right facing arrow. | |
| To the right, and slightly above the arrow is the cyanide ion however, the electron pair on the carbon has been deleted as has the negative charge. Instead a bond is drawn from the carbon to an H. Below and slightly to the right of the arrow is a copy of the ethanol structure. However, 6 electron dots have been added, the bond between the O and H, as well as the H have been deleted, and a negative charge has been added. To the right of this structure is an Na with a positive charge. | The student shows the products of the deprotonation of ethanol by cyanide: hydrocyanic acid and sodium ethoxide. |

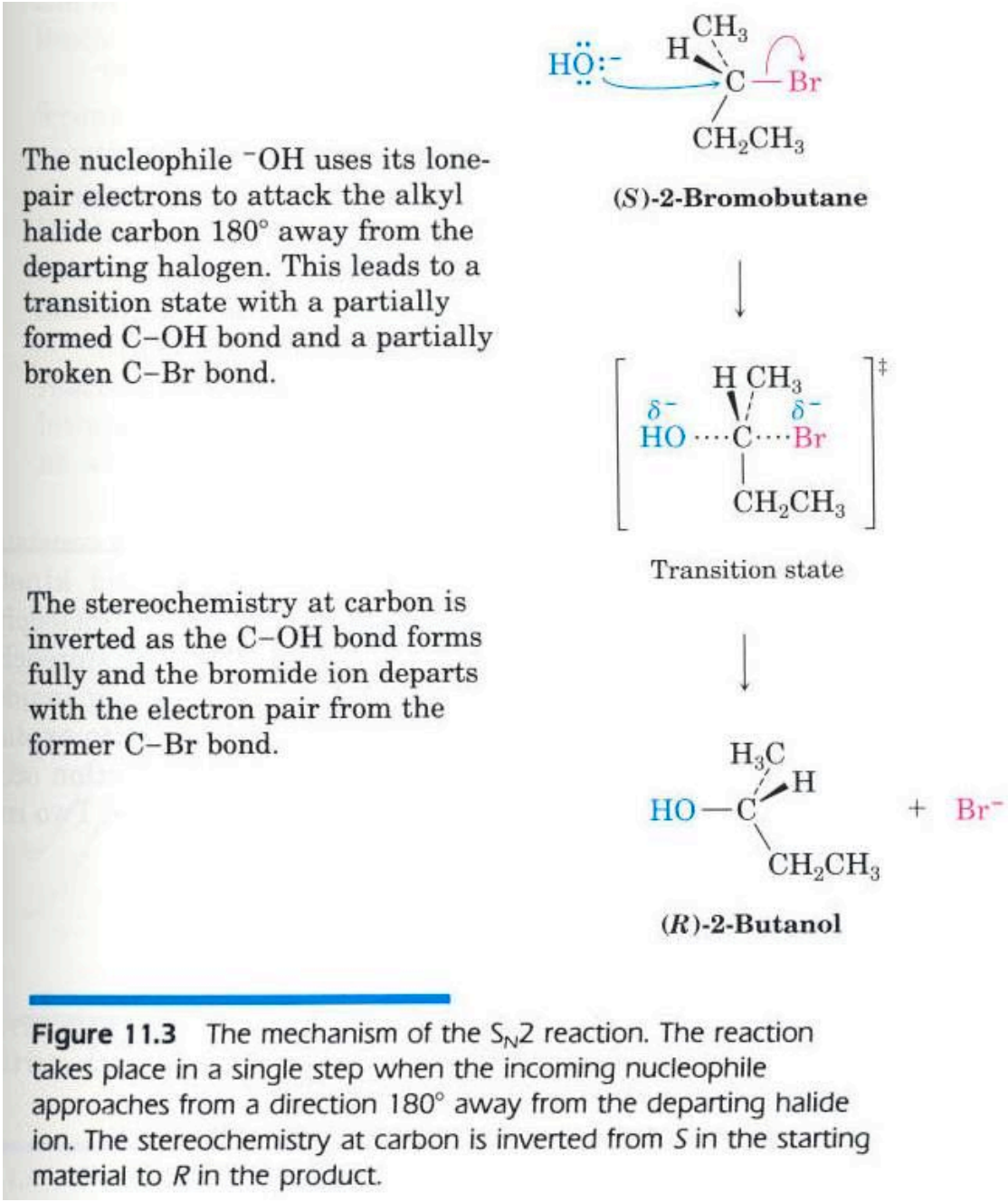


**Figure 11.3** The mechanism of the $S_N2$ reaction. The reaction takes place in a single step when the incoming nucleophile approaches from a direction 180° away from the departing halide ion. The stereochemistry at carbon is inverted from *S* in the starting material to *R* in the product.

File: McMurray SN2(legend).jpg
McMurry, J. (1992). *Organic Chemistry* (3rd ed.). Belmont, CA: Brooks/Cole Publishing Co., p. 365.

| Verbal Transcription | Translation/Interpretation |
|---|---|

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| The entire drawing is written as a series of 3 pictures drawn vertically. On the right side of the figure are the drawings, and on the left side are two sections of descriptive text.<br><br>The first set of text reads, "The nucleophile -OH uses its lone-pair electrons to attack the alkyl halide carbon 180° away from the departing halogen. This leads to a transition state with a partially formed C-OH bond and a partially broken C-Br bond."<br><br>The second set of text reads, "The stereochemistry at carbon is inverted as the C-OH bond forms fully and the bromide ion departs with the electron pair from the former C-Br bond."<br><br>The caption reads, "The mechanism of the $S_N2$ reaction. The reaction takes place in a single step when the incoming nucleophile approaches from a direction 180° away from the departing halide ion. The stereochemistry at carbon is inverted from S in the starting material to R in the product." | |
| The top picture is a blue hydroxide ion indicated by an HO. The O has 6 dots around it and a negative charge. | Hydroxide anion |
| To the right of the HO is a carbon atom with 4 attached groups, an H, a $CH_3$, and a $CH_2CH_3$, and a pink Br. Stereochemistry is indicated. The compound is labeled (S)-2-bromobutane. | (S)-2-bromobutane |
| Below the (S)-2-bromobutane is a downward pointing arrow. | yields |
| Below the arrow is a blue hydroxide group indicated by an HO connected with a dotted line to the C of the 2-bromobutane. The pink Br is now connected to the C with a dotted line and the other groups have shifted to the right of the picture. There is a blue δ- above the blue HO and a blue δ- above the pink Br. There are two large | A transition state where the geometry around the central carbon is in the process of inverting while bond making and bond breaking take place. The hydroxide anion is becoming less negative as it donates electrons to the carbon and the bromide anion is becoming more negative as it leaves |

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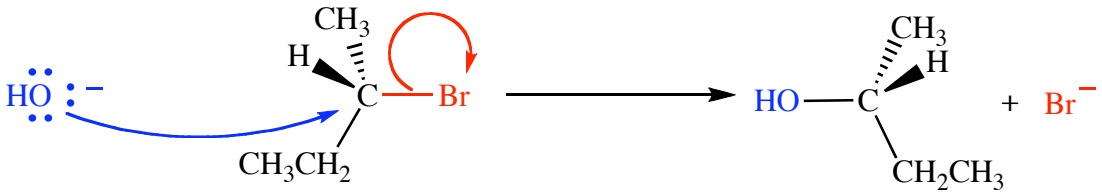
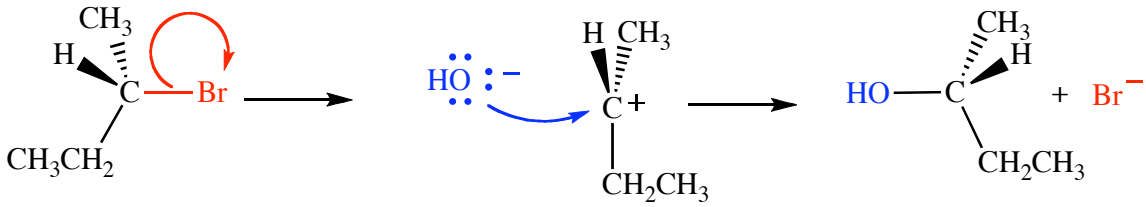
| brackets surrounding the picture and "‡" symbol. Below the drawing is the label "Transition state". | |
| Below the "Transition state" drawing is a downward facing arrow. | Yields |
| Below the arrow is a carbon atom with 4 attached groups, an H, a $CH_3$, and a $CH_2CH_3$, and a blue OH on the left side. Stereochemistry is indicated. The compound is labeled "(R)-2-Butanol". | (R)-2-butanol |
| To the right of the (R)-2-Butanol is a plus sign. | and |
| To the right of the plus sign is a pink Br with a negative charge. | Bromide anion |
| There is a blue, curved, right facing that extends from the O of the first hydroxide anion toward the C of the carbon group. | The oxygen atom of the hydroxide anion attacks the carbon atom of (S)-2-bromobutane. |
| There is a pink, curved, right facing arrow which extends from the line between the carbon group and Br toward the Br. | The bromide anion leaves (S)-2-bromobutane. |




(*S*)-2-Bromobutane (*R*)-2-Butanol

File: SN1-SN2mockups.cdx
SN2 mechanism without transition state. Based on McMurry, J. (1992). *Organic Chemistry* (3rd ed.). Belmont, CA: Brooks/Cole Publishing Co., p. 365.

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The entire drawing is written a series of 2 pictures drawn horizontally. | |
| On the far left is a picture of a blue hydroxide ion indicated by an HO. The O has 6 dots around it and a negative charge. | Hydroxide anion |
| To the right of the HO is a carbon atom with 4 attached groups, an H, a $CH_3$, and a $CH_2CH_3$, and a pink Br. Stereochemistry is indicated. The compound is labeled (S)-2-bromobutane. | (S)-2-bromobutane |
| To the right of the (S)-2-bromobutane is a rightward pointing arrow. | yields |
| To the right of the the arrow is a carbon atom with 4 attached groups, an H, a $CH_3$, and a $CH_2CH_3$, and a blue OH on the left side. Stereochemistry is indicated. The compound is labeled "(R)-2-Butanol". | (R)-2-butanol |
| To the right of the (R)-2-Butanol is a plus sign. | and |
| To the right of the plus sign is a pink Br with a negative charge. | Bromide anion |
| There is a blue, curved, right facing that extends from the O of the first hydroxide anion toward the C of the carbon group. | The oxygen atom of the hydroxide anion attacks the carbon atom of (S)-2-bromobutane. |
| There is a pink, curved, right facing arrow which extends from the line between the carbon group and Br toward the Br. | The bromide anion leaves (S)-2-bromobutane. |



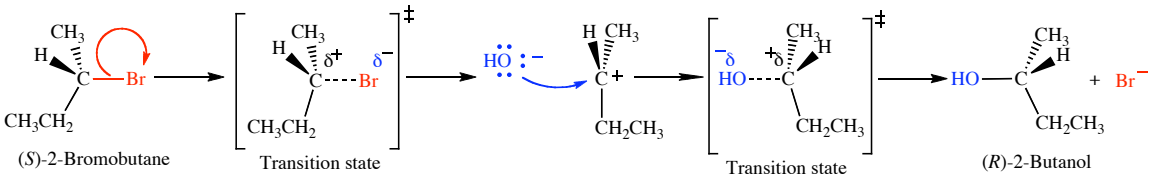

(*S*)-2-Bromobutane (*R*)-2-Butanol

File: SN1-SN2mockups.cdx

SN1-like mechanism with intermediate but without transition state. Based on McMurry, J. (1992). *Organic Chemistry* (3rd ed.). Belmont, CA: Brooks/Cole Publishing Co., p. 365.

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The entire drawing is written a series of 3 pictures drawn horizontally. | |
| On the far right is a carbon atom with 4 attached groups, an H, a $CH_3$, and a $CH_2CH_3$, and a pink Br. Stereochemistry is indicated. The compound is labeled (S)-2-bromobutane. | (S)-2-bromobutane |
| To the right of the (S)-2-bromobutane is a rightward pointing arrow. | yields |
| To the right of the arrow is a blue hydroxide ion indicated by an HO. The O has 6 dots around it and a negative charge. | Hydroxide anion |
| To the right of the HO is a carbon atom with 3 attached groups, an H, a $CH_3$, and a $CH_2CH_3$. There is a positive charge next to the carbon atom. Planar geometry is indicated. | Carbocation intermediate |
| To the right of the carbocation is a rightward pointing arrow. | yields |
| To the right of the arrow is a carbon atom with 4 attached groups, an H, a $CH_3$, and a $CH_2CH_3$, and a blue OH on the left side. Stereochemistry is indicated. The compound is labeled "(R)-2-Butanol." | (R)-2-butanol |
| To the right of the (R)-2-Butanol is a plus sign. | and |
| To the right of the plus sign is a pink Br with a negative charge. | Bromide anion |
| There is a pink, curved, right facing arrow which extends from the line between the carbon group and Br toward the Br. | The bromide anion leaves (S)-2-bromobutane. |
| There is a blue, curved, right facing that extends from the O of the first hydroxide | The oxygen atom of the hydroxide anion attacks the carbon atom of the carbocation. |

| | |
|---|---|
| anion toward the C of the carbon group. | |




File: SN1-SN2mockups.cdx
SN1-like mechanism with intermediate and transition states. Based on McMurry, J. (1992). *Organic Chemistry* (3rd ed.). Belmont, CA: Brooks/Cole Publishing Co., p. 365.

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The entire drawing is written a series of 5 pictures drawn horizontally. | |
| On the far right is a carbon atom with 4 attached groups, an H, a $CH_3$, and a $CH_2CH_3$, and a pink Br. Stereochemistry is indicated. The compound is labeled (S)-2-bromobutane. | (S)-2-bromobutane |
| To the right of the (S)-2-bromobutane is a rightward facing arrow. | yields |
| To the right of the arrow is carbon atom with 4 attached groups, an H, a $CH_3$, and a $CH_2CH_3$, and a pink Br. The pink Br is now connected to the C with a dotted line and the other groups have shifted to the right of the picture. There is a δ+ next to the carbon atom and a blue δ- above the pink Br. There are two large brackets surrounding the picture and "‡" symbol. Below the drawing is the label "Transition state." | A transition state where the geometry around the central carbon is in the process of inverting while bond breaking takes place. The carbon atom is becoming more positive as it donates electrons to the bromine atom and the bromide anion is becoming more negative as it leaves |
| To the right of the "Transition state" drawing is a rightward facing arrow. | yields |
| To the right of the arrow is a picture of a blue hydroxide ion indicated by an HO. The O has 6 dots around it and a negative charge. | Hydroxide anion |
| To the right of the HO is a carbon atom with 3 attached groups, an H, a $CH_3$, and a $CH_2CH_3$. There is a positive charge next to the carbon atom. Planar geometry is indicated. | Carbocation intermediate |
| To the right of the carbon atom with 3 attached groups is a rightward facing arrow. | yields |
| To the right of the arrow is carbon atom with 4 attached groups, an H, a $CH_3$, and a | A transition state where the geometry around the central carbon is in the process |

| | |
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| $CH_2CH_3$, and a blue HO. The blue HO is now connected to the C with a dotted line and the other groups have shifted to the right of the picture. There is a δ+ next to the carbon atom and a blue δ- above the blue HO. There are two large brackets surrounding the picture and "‡" symbol. Below the drawing is the label "Transition state." | of inverting while bond breaking takes place. The carbon atom is becoming less positive as it accepts electrons from the hydroxide anion and the hydroxide anion is becoming less negative as it forms a bond with the carbon atom. |
| To the right of the "Transition state" drawing is a rightward facing arrow. | yields |
| To the right of the arrow is a carbon atom with 4 attached groups, an H, a $CH_3$, and a $CH_2CH_3$, and a blue OH on the left side. Stereochemistry is indicated. The compound is labeled "(R)-2-Butanol". | (R)-2-butanol |
| To the right of the (R)-2-Butanol is a plus sign. | and |
| To the right of the plus sign is a pink Br with a negative charge. | Bromide anion |
| There is a pink, curved, right facing arrow which extends from the line between the carbon group and Br toward the Br. | The bromide anion leaves (S)-2-bromobutane. |
| There is a blue, curved, right facing that extends from the O of the first hydroxide anion toward the C of the carbon group. | The oxygen atom of the hydroxide anion attacks the carbon atom of the carbocation. |

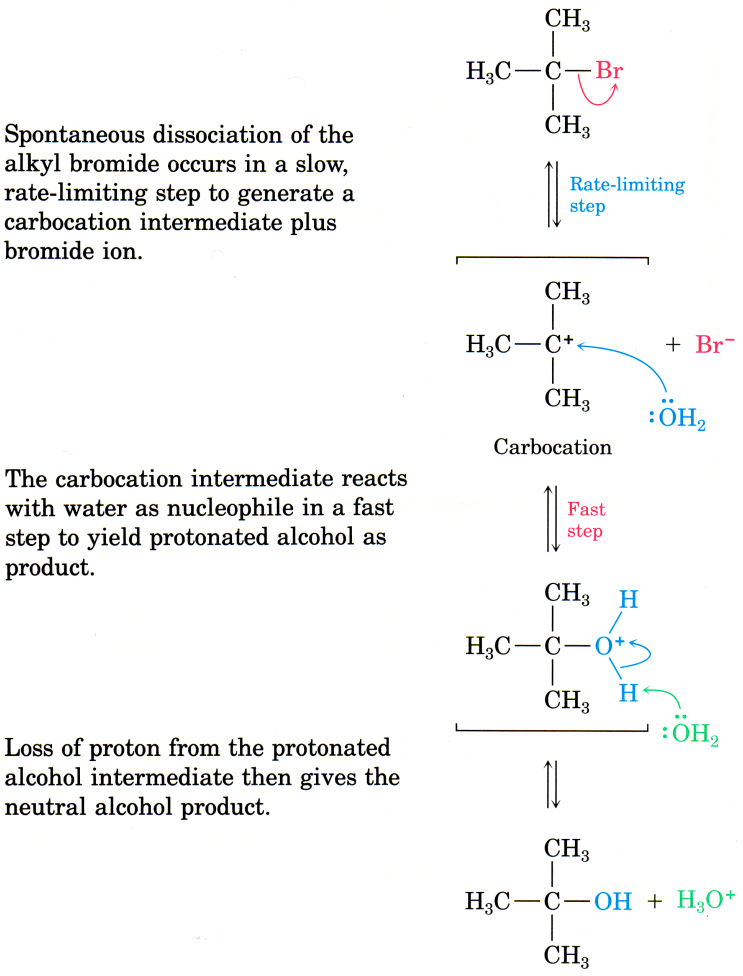


**Figure 11.10** The mechanism of the $S_N1$ reaction of 2-bromo-2-methylpropane with water. Three steps are involved, with the first one rate-limiting.

McMurry, J. (1992). *Organic Chemistry* (3rd ed.). Belmont, CA: Brooks/Cole Publishing Co., p. 365.

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The entire drawing is written a series of 4 pictures drawn vertically. On the right side of the figure are the drawings, and on the left side are three sections of text, written descriptions.<br><br>The first section of text reads, "Spontaneous dissociation of the alkyl bromide occurs in a slow, rate-limiting step | |

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| to generate a carbocation intermediate plus bromide ion."<br><br>The second section of text reads, "The carbocation intermediate reacts with water as nucleophile in a fast step to yield protonated alcohol as product."<br><br>The third section of text reads, "Loss of proton from the protonated alcohol intermediate then gives the neutral alcohol product."<br><br>The caption reads, "The mechanism of the $S_N1$ reaction of 2-bromo-2-methylpropane with water. Three steps are involved, with the first one rate-limiting." | |
| The top picture is a carbon atom connected with 3 lines to 3 $CH_3$ groups and one pink Br. | 2-bromo-2-methylpropane |
| Below the first drawing is a set of downward facing equilibrium arrows labeled "Rate-limiting step" in blue. | Yields in a rate-limiting step |
| Below the arrows is a carbon atom connected with 3 lines to 3 $CH_3$ groups and a positive charge on the C. This structure is labeled "carbocation." Below the carbocation is a blue $OH_2$ with electrons around the O. This drawing and the one below it are contained within brackets. | The carbocation is an intermediate. The carbocation reacts with water. |
| To the right of the carbon atom connected with 3 lines to 3 $CH_3$ groups and a positive charge on the C is a plus sign | and |
| To the right of the plus sign is pink Br with a negative charge. | Bromide anion |
| Below the carbocation is a set of downward facing equilibrium arrows labeled "Fast step" in pink. | Yields in a fast step. |
| Below the equilibrium arrows is a carbon atom connected with 3 lines to 3 $CH_3$ groups and one blue O. The O is connected with two blue lines to two blue H's and has a blue positive charge. Below this drawing is a green $OH_2$ with 2 sets of electrons. | Protonated 2-methylpropanol cation intermediate reacts with water |
| Below the propanol intermediate is a set of | yields |

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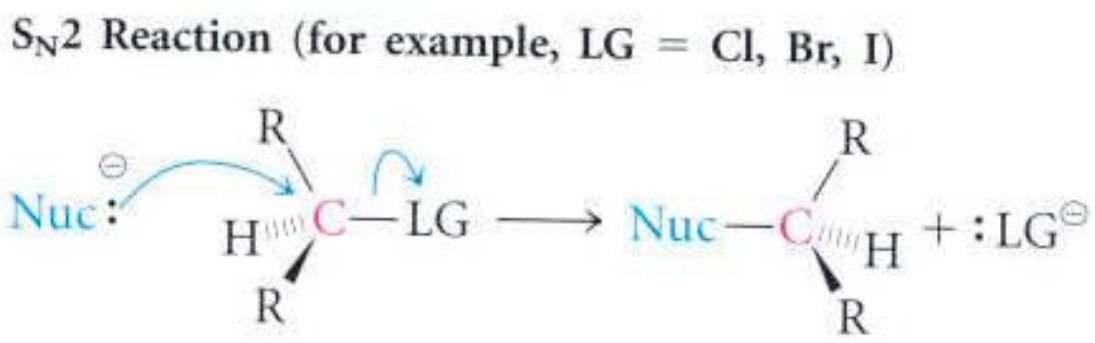
| downward facing equilibrium arrows. | |
| Below the equilibrium arrows is a carbon atom connected with 3 lines to 3 $CH_3$ groups and one blue OH. | 2-methylpropanol |
| To the right of the carbon atom connected with 3 lines to 3 $CH_3$ groups and one blue OH is a plus sign. | and |
| To the right of the plus sign is a green $H_3O$ with a positive charge | Hydronium cation. |
| There is a pink, curved, right facing arrow that extends from the C of the carbon group toward the pink Br. | The bromide atom leaves in a heterolytic cleavage |
| There is a blue, curved, left facing arrow that extends from the blue $OH_2$ toward the C of the carbocation intermediate. | Water reacts with the carbocation |
| There is a blue, curved, left facing arrow that extends from the line between the O and one of the blue H's on the second intermediate toward the O. | The cation is deprotonated |
| There is a green, curved, left facing arrow that extends from the green $OH_2$ toward one of the blue H's on the second intermediate | Water deprotonates the second intermediate |

file: Bruice SN2.jpg
Bruice, P. Y. (1998). *Organic Chemistry* (2nd ed.). Upper Saddle River, NJ: Simon & Schuster, p 361.

| Verbal Transcription | Translation/Interpretation |
|---|---|
| The entire drawing is written as an equation on one line. On the left most side of the picture is a hydroxide ion indicated by HO. The O has 6 dots around it and a negative charge. | Hydroxide anion |
| To the right of the hydroxide ion is a plus sign. | and |
| To the right of the plus sign is a methyl group indicated by $CH_3$. A line is drawn between the $CH_3$ and a Br. The Br has six dots around it. | Methyl bromide |
| To the right of the methyl bromide is right facing arrow. | yields |
| To the right of the arrow is a methyl group indicated by $CH_3$. A line is drawn between the $CH_3$ and OH. | Methanol |
| To the right of the OH is a plus sign. | and |
| To the right of the plus sign is a bromine ion indicated by Br. There are 8 dots around it and a negative charge. | Bromide anion |
| There is a red, curved, right facing arrow, which extends from the O of the first hydroxide ion toward the C of the first methyl group. | The oxygen atom of the hydroxide anion is shown attacking the carbon atom of methyl bromide. |
| There is a red, curved, right facing arrow which extends from the line between the methyl group and Br toward the Br. | The bromide anion leaves methyl bromide. |




File: Fox SN2 (all).jpg
Fox, M. A., & Whitesell, J. K. (2004). *Organic Chemistry* (3rd ed.). Sudbury, MA: Jones and Bartlett, p 372.

| Verbal Transcription | Translation/Interpretation |
|---|---|
| At the top of the drawing are the words, "$S_N2$ Reaction (for example, LG = Cl, Br, I) | The reaction is labeled as $S_N2$, and the LG is shown as a placeholder for Cl, Br, or I groups. |
| The entire drawing is written as an equation on one line. On the left most side of the picture is the abbreviation "Nuc" in blue. The "Nuc" has 2 dots to the left of it and a negative charge. | Negatively charged nucleophile with a lone pair of electrons. |
| To the right of the "Nuc" is a carbon atom with 4 substituents: two are R groups, one is an H group and one is an "LG" group, shown on the left side of the carbon. The C is shown with tetrahedral geometry. The C is red. | A general methyl, 1˚, or 2˚ carbon group is shown with tetrahedral geometry. |
| To the right of the methyl bromide is right facing arrow. | yields |
| To the right of the arrow is a carbon atom with 4 substituents: two are R groups, one is an H group and one is a blue "Nuc" group, which is shown on the right side of the carbon. The C is shown with tetrahedral stereochemistry. | The nucleophile has replaced the leaving group and the tetrahedral geometry has inverted. |
| To the right of the carbon group is a plus sign. | and |
| To the right of the plus sign is the abbreviation "LG". There are 2 dots to the right of it and a negative charge. | Negatively charged leaving group with a lone pair of electrons. |
| There is a blue, curved, right facing arrow that extends from the dots on the "Nuc" toward the C on the right side of the | The nucleophile attacks the carbon atom of the carbon group. |

| | |
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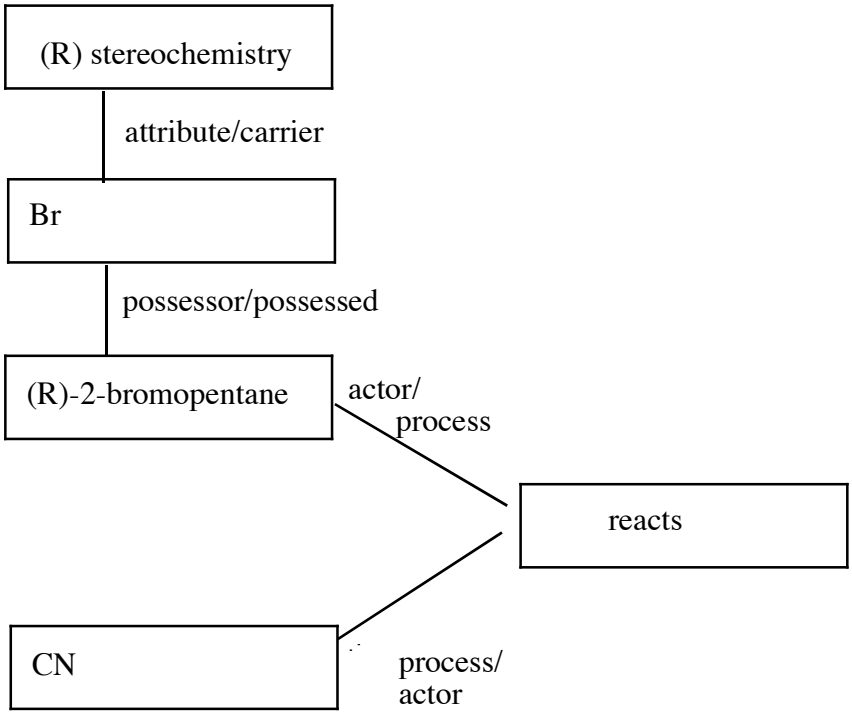
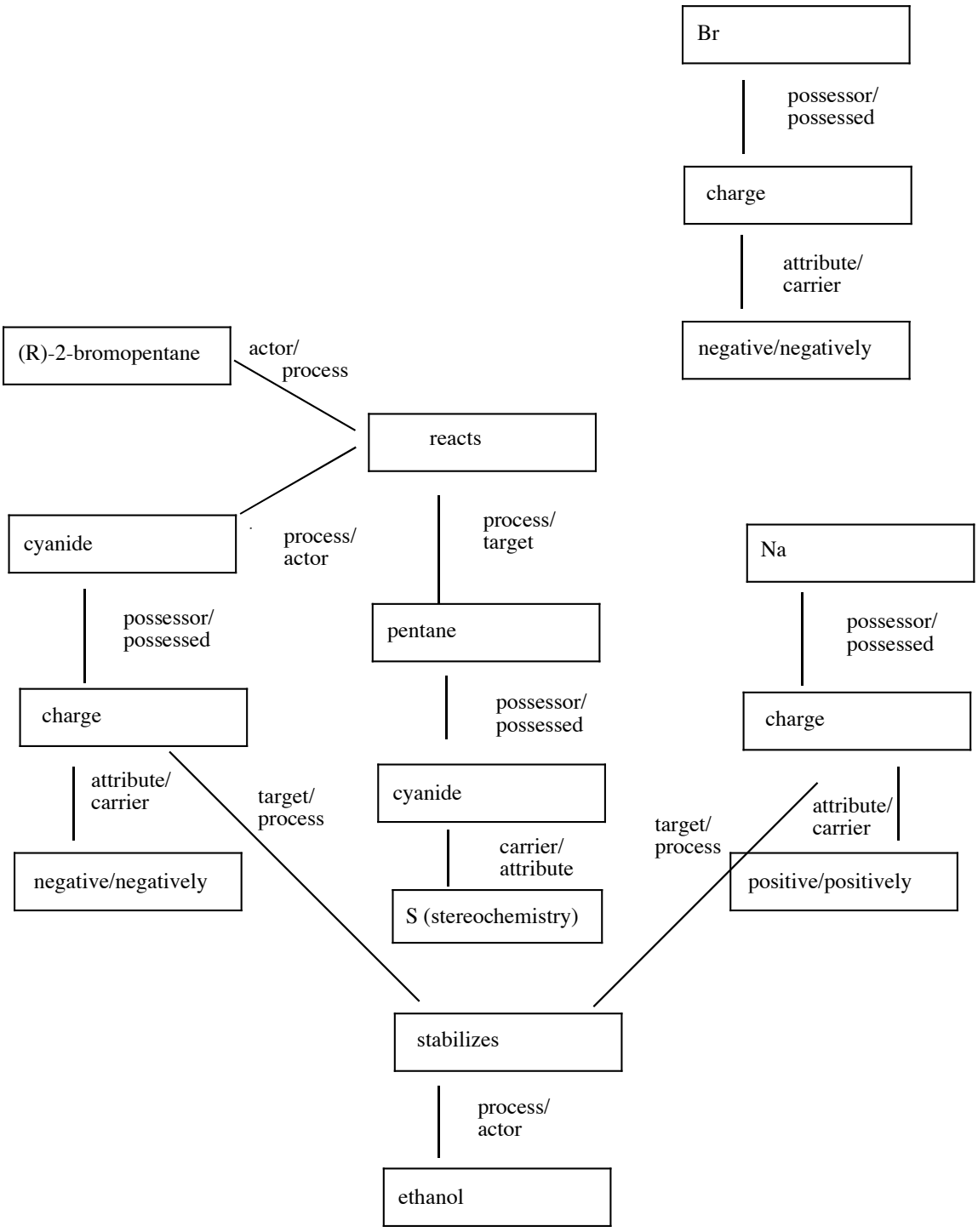
| equation. | |
| There is a blue, curved, right facing arrow which extends from the line between the carbon and the "LG" toward the LG. | The leaving group leaves. |

# APPENDIX B: THEMATIC MAPS

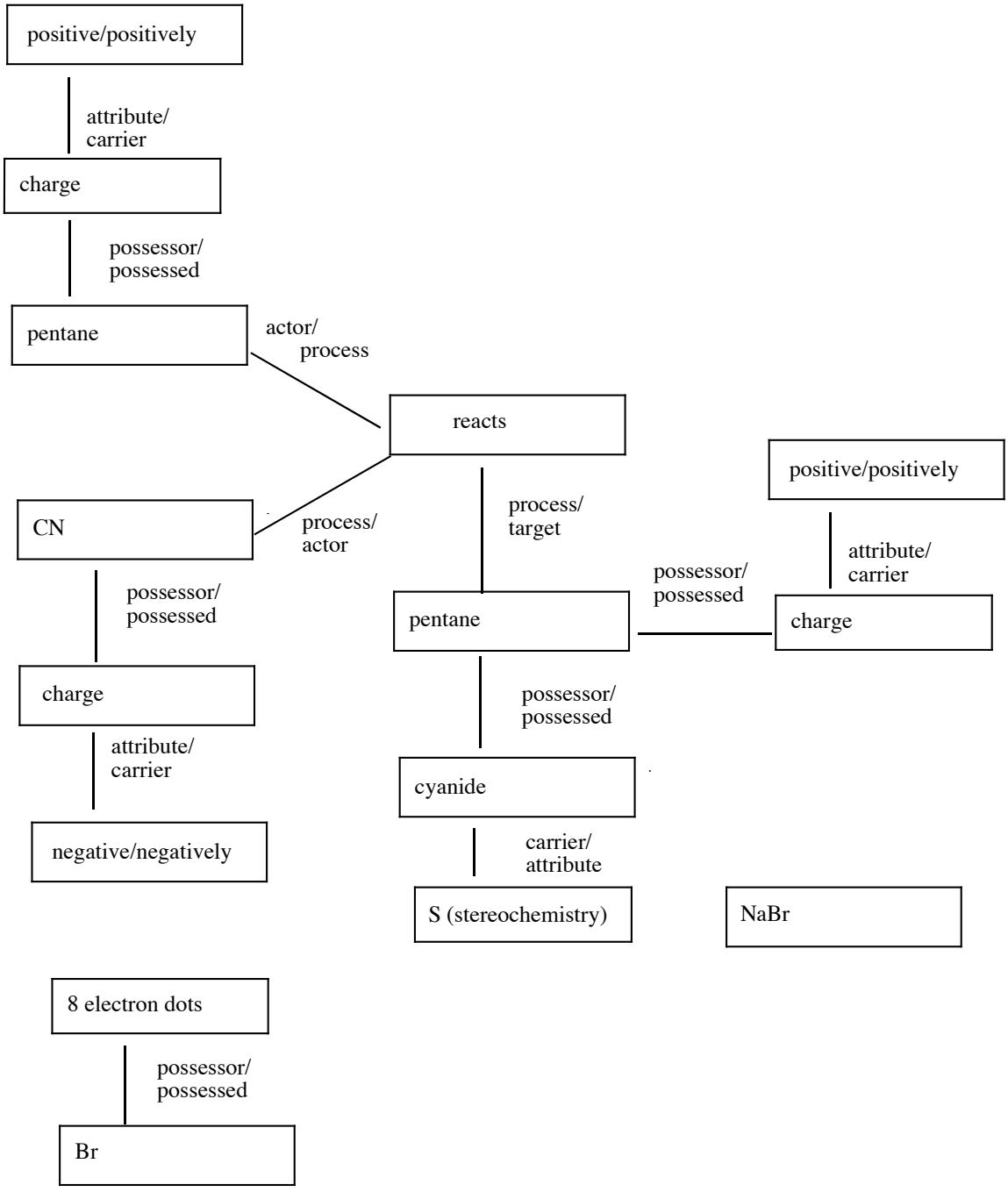
## Thematic Diagram for visual file wk8S,MC



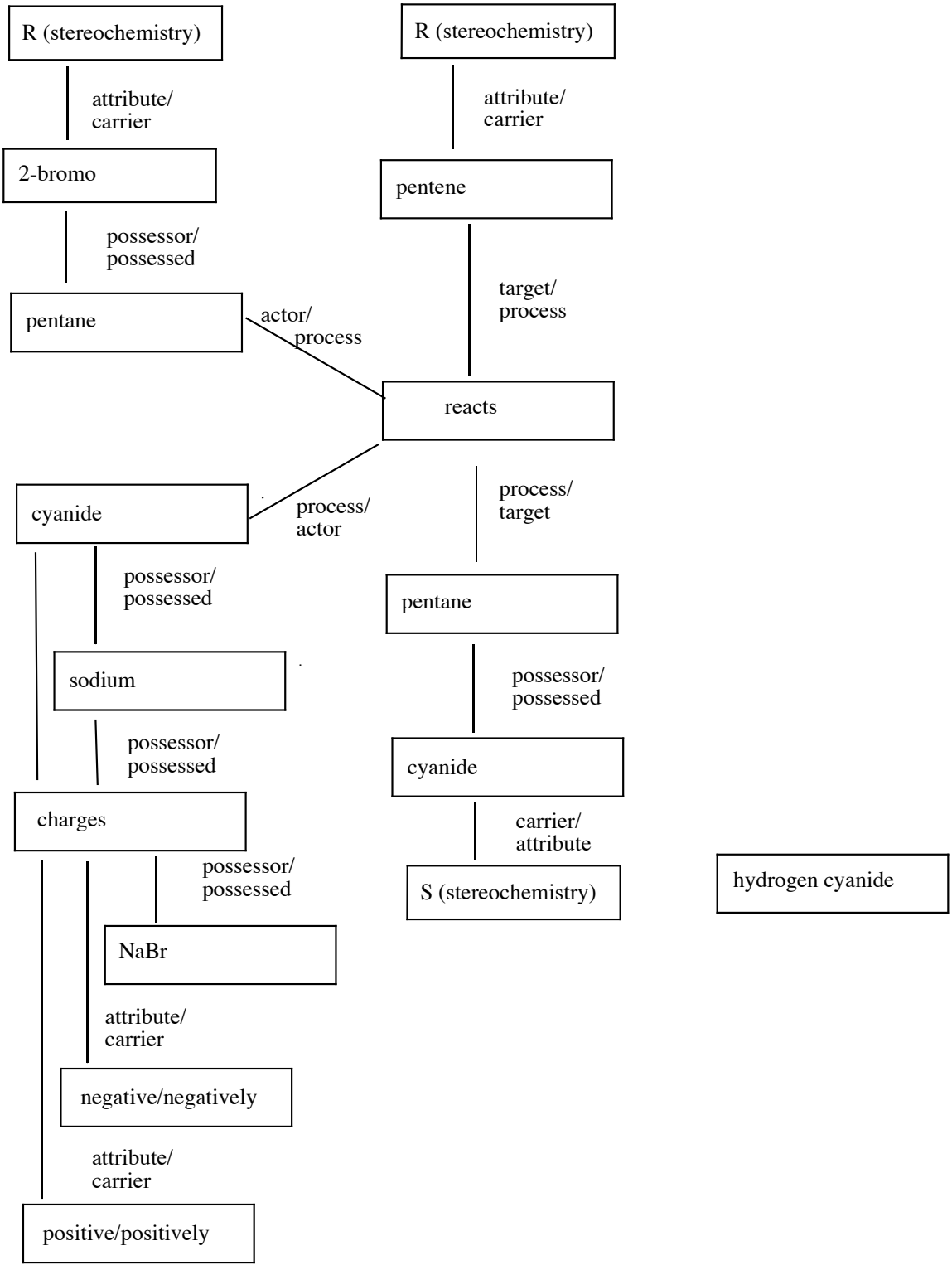
**Thematic Diagram for visual file wk8Se,S**



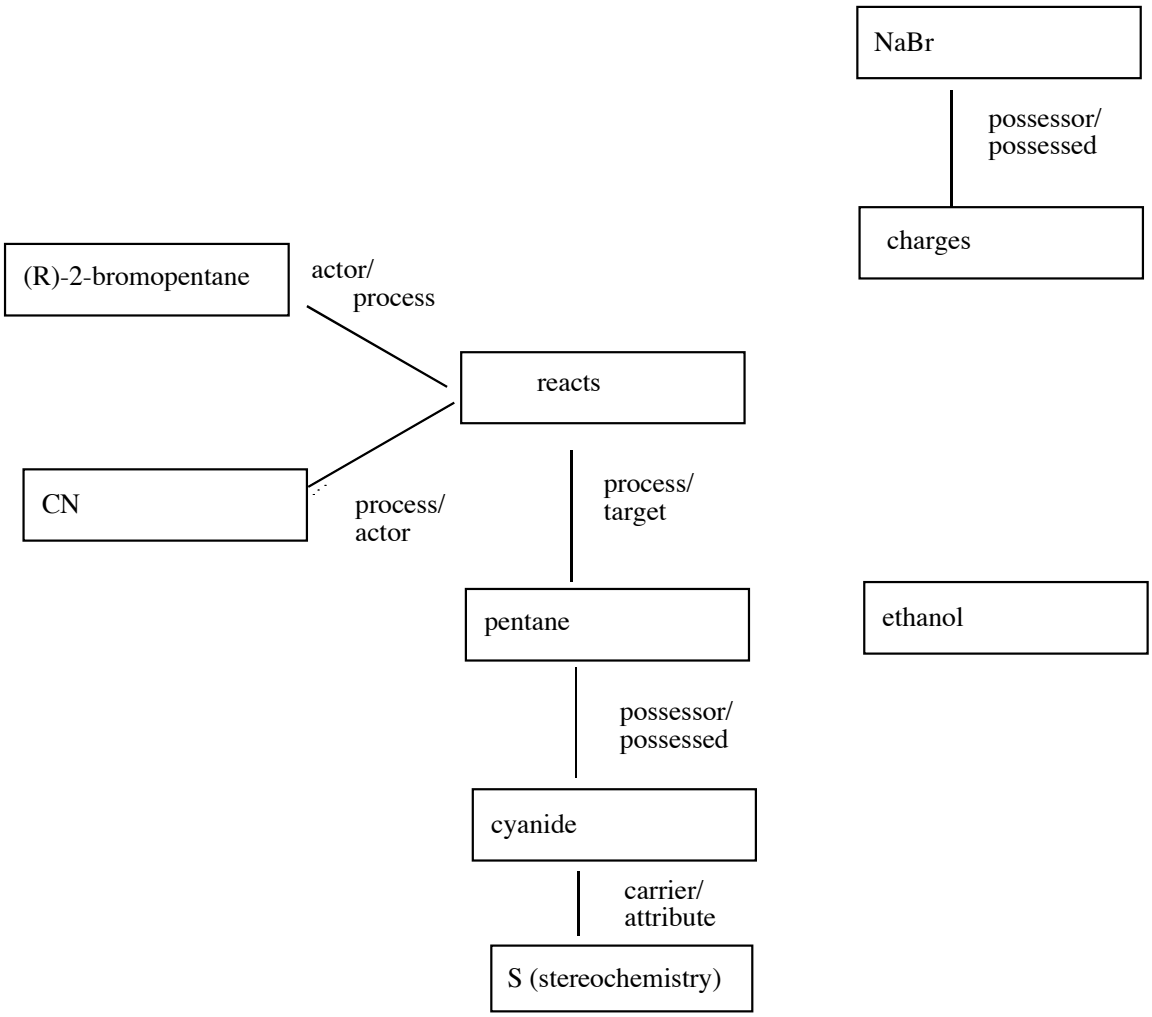
**Thematic Diagram for visual file wk8N,AT**



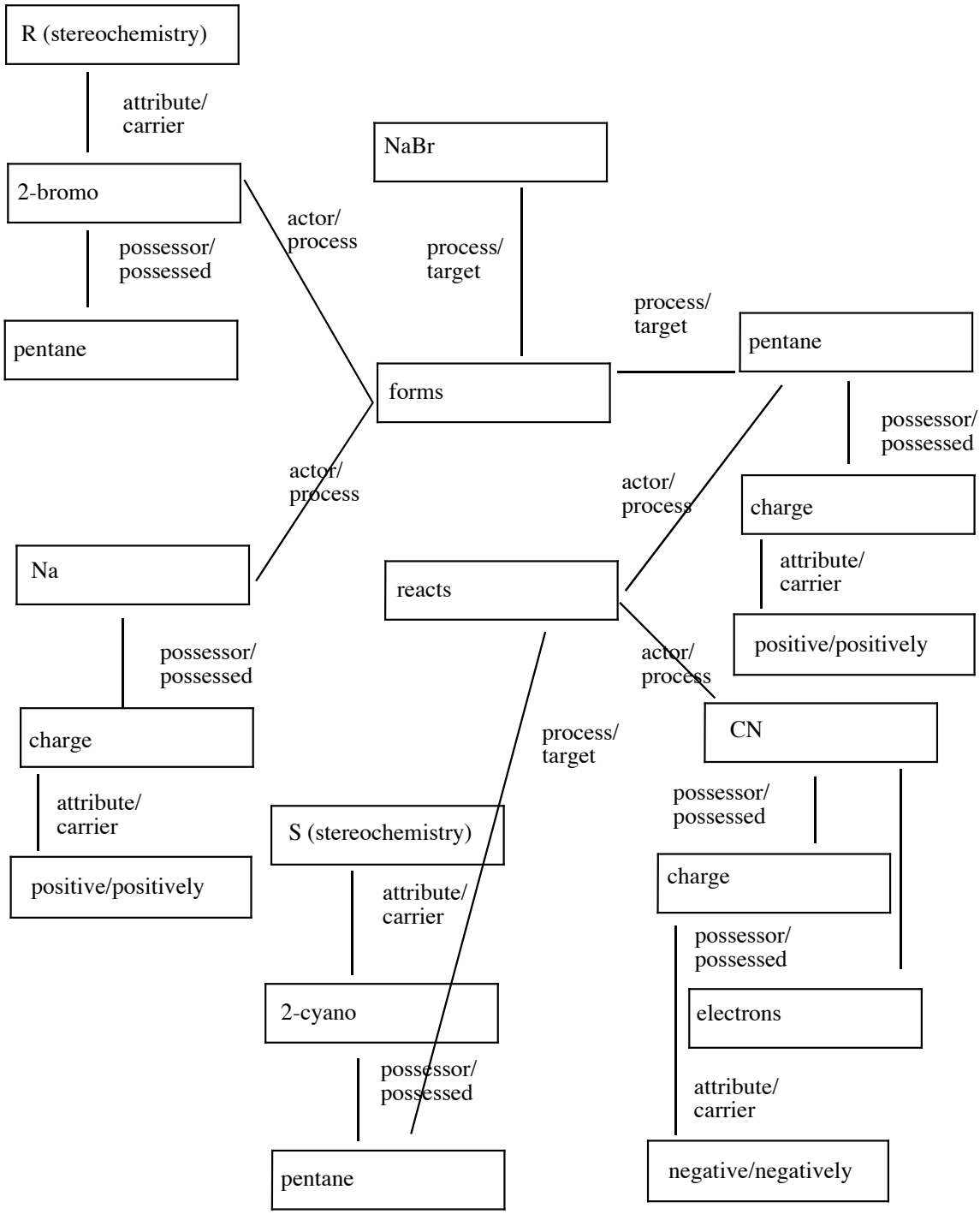
**Thematic Diagram for visual file wk8N,J**



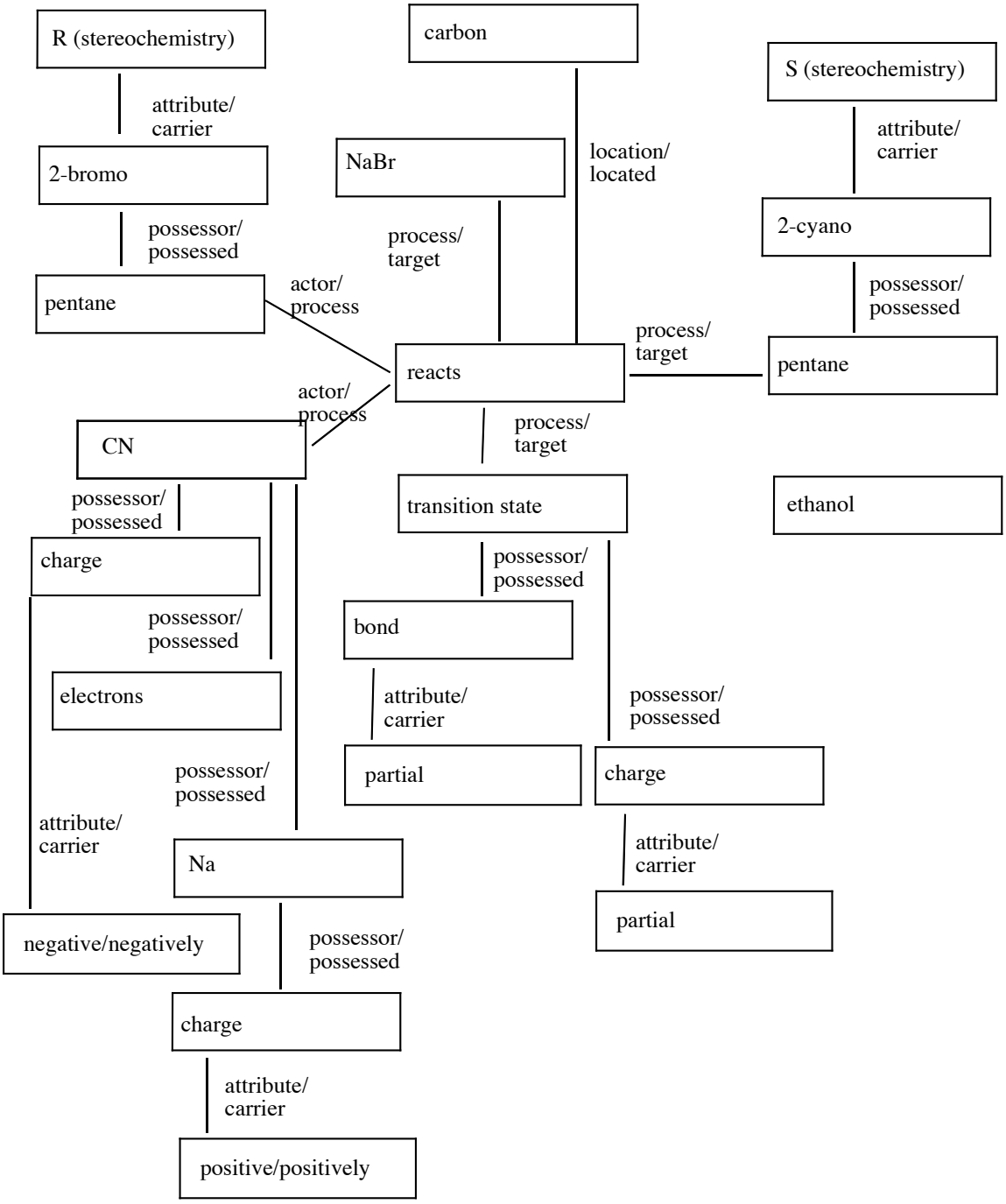
**Thematic Diagram for visual file wk8N,JM**



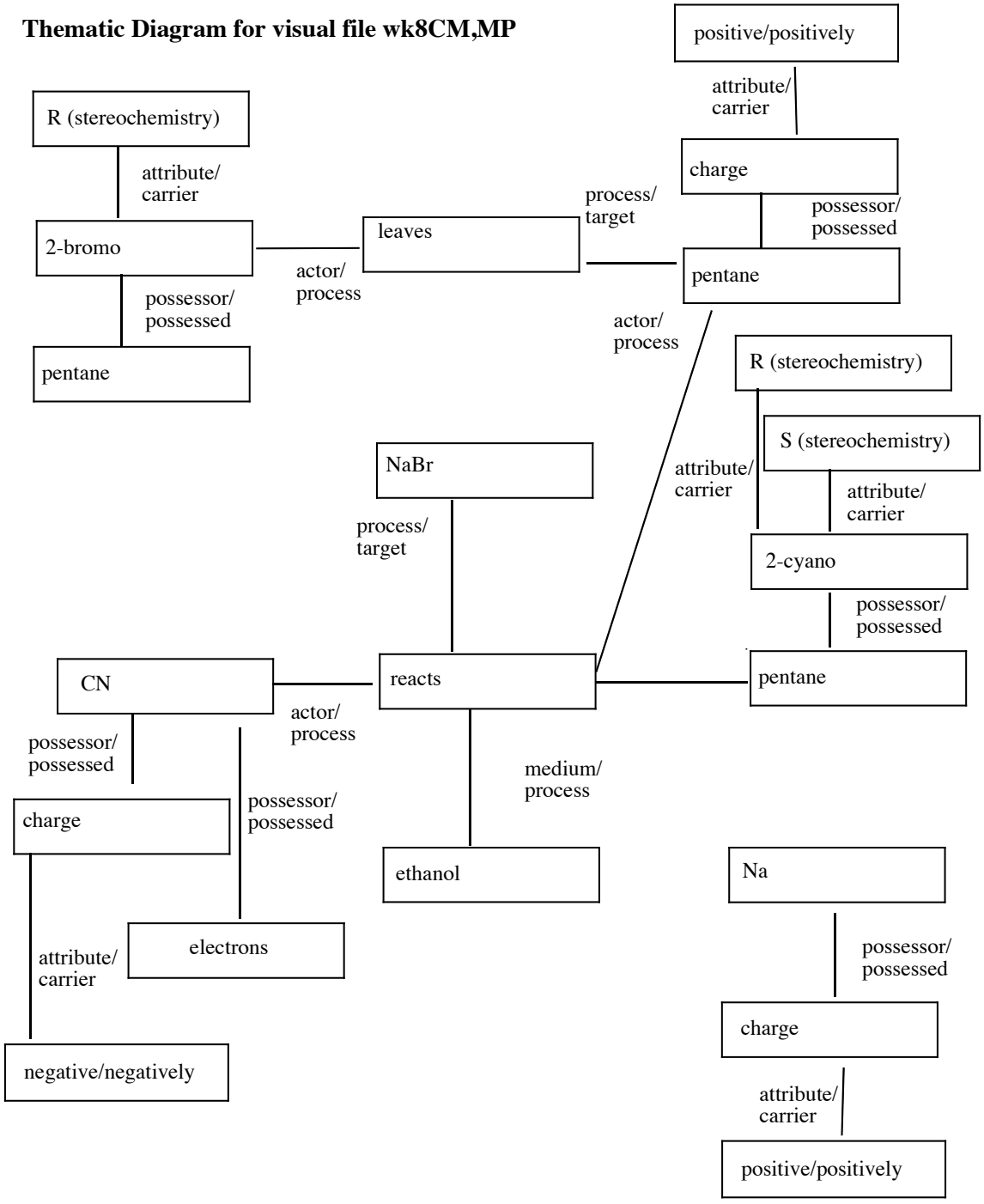
**Thematic Diagram for visual file wk8AP,KZ**



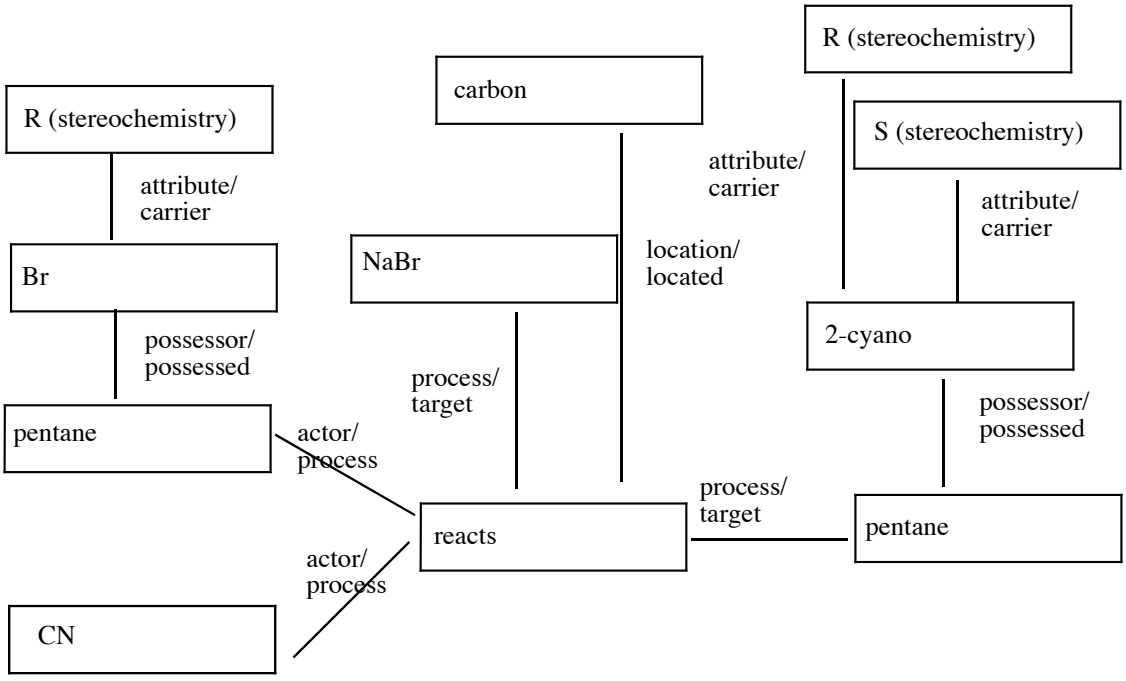
**Thematic Diagram for visual file wk8CM,EF**



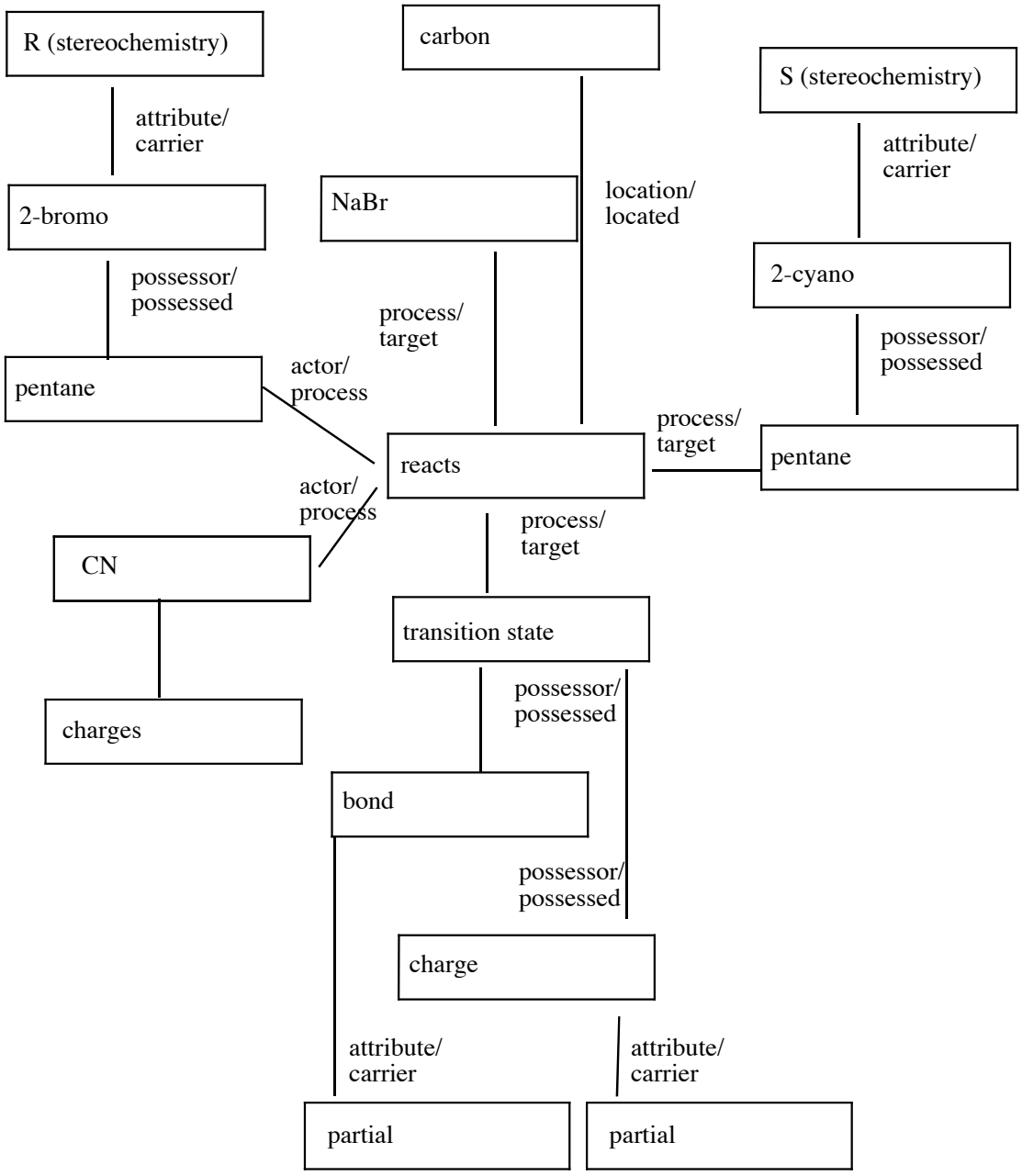
**Thematic Diagram for visual file wk8CM,MP**



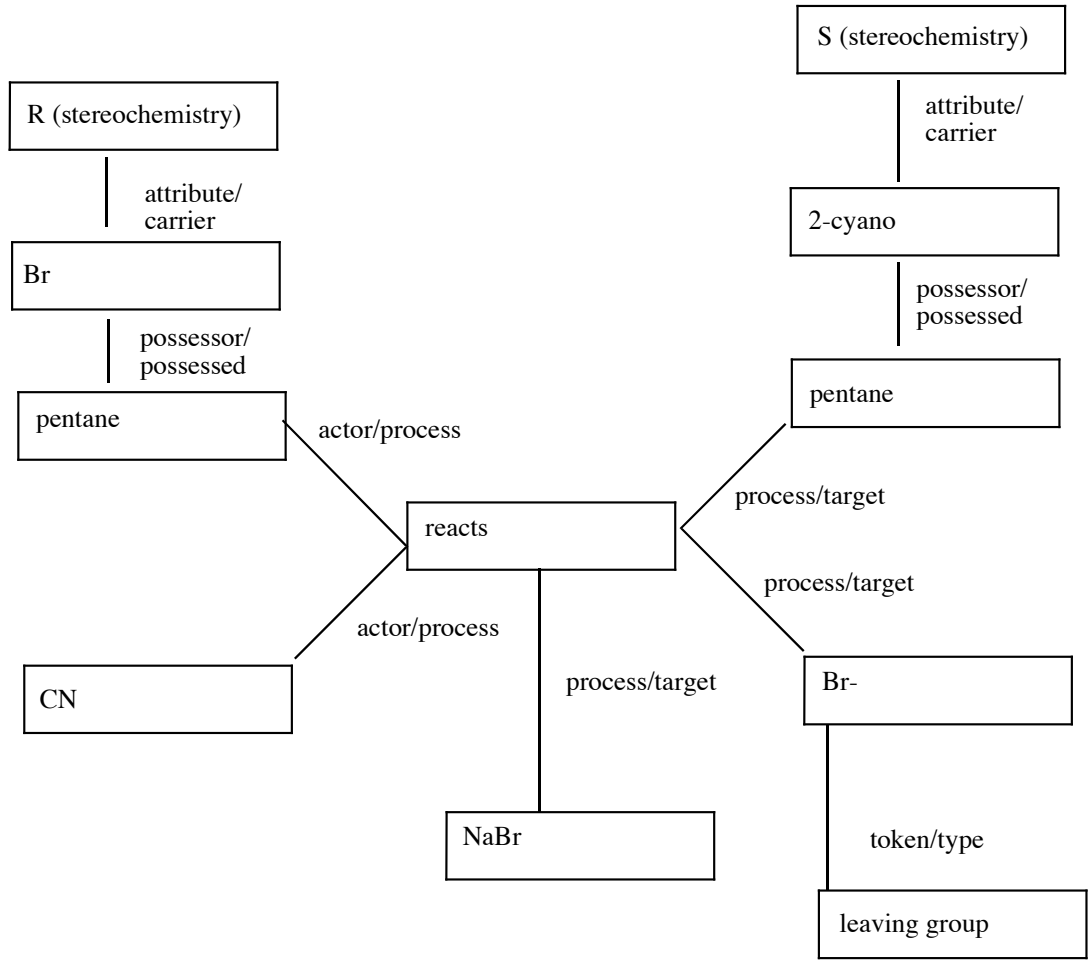
**Thematic Diagram for visual file wk8DB,ES**



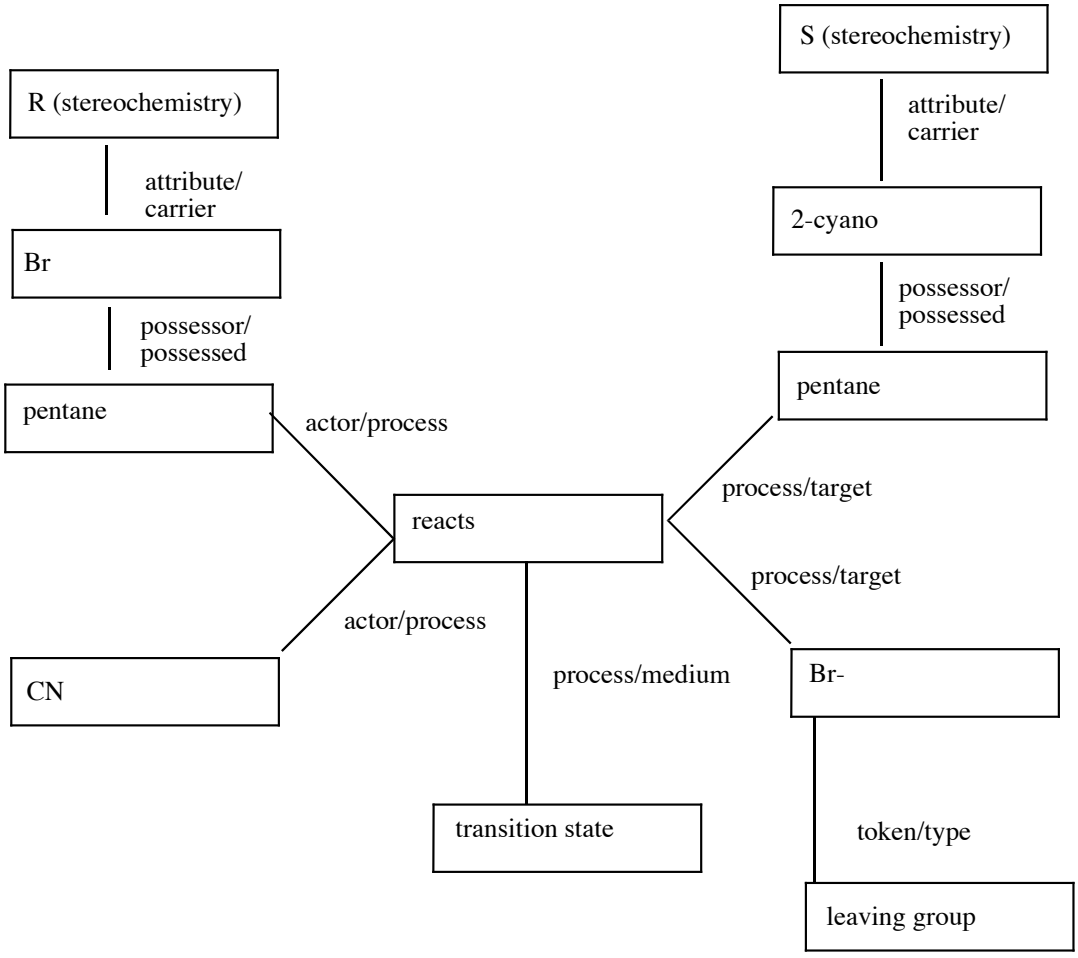
**Thematic Diagram for visual file wk8DB,KK**



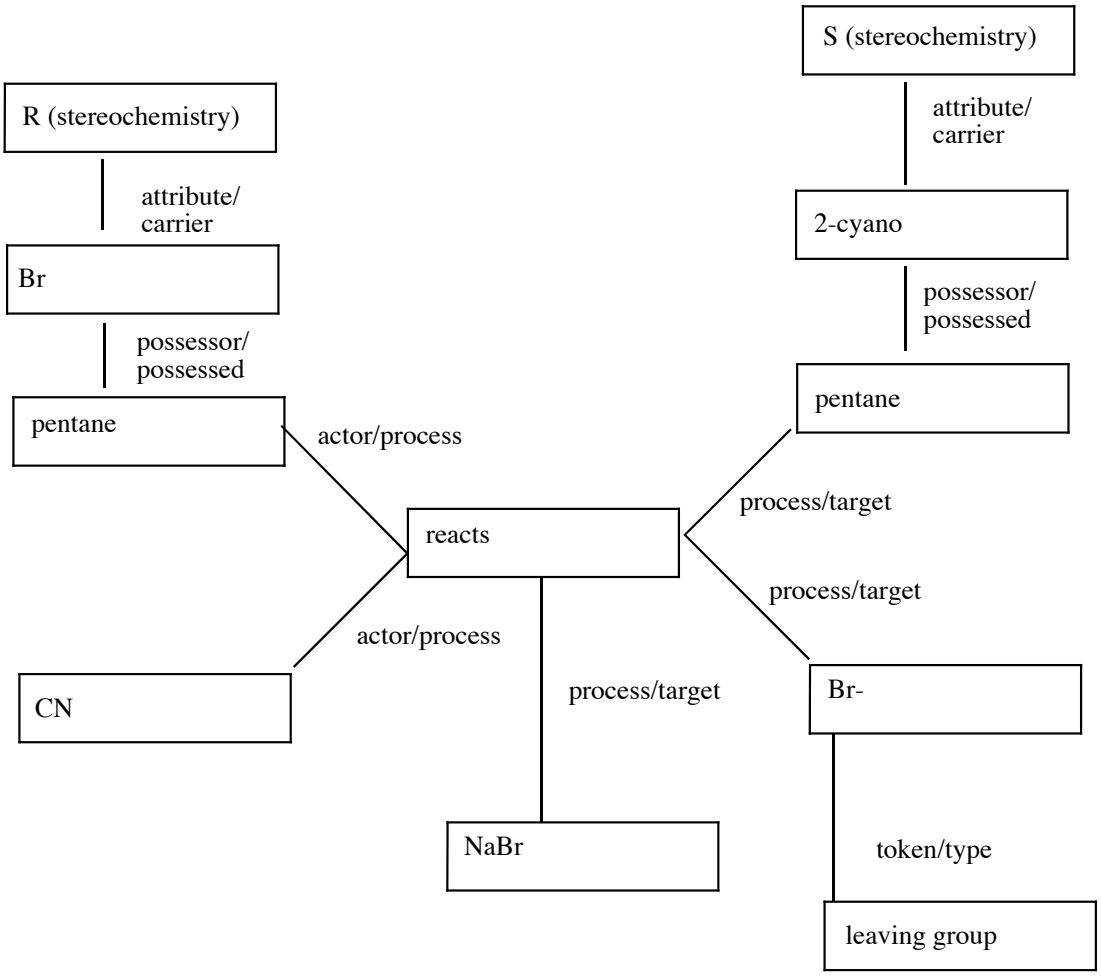
**Thematic Diagram for visual file wk8AdvSR**



**Thematic Diagram for visual file wk8AdvWG**

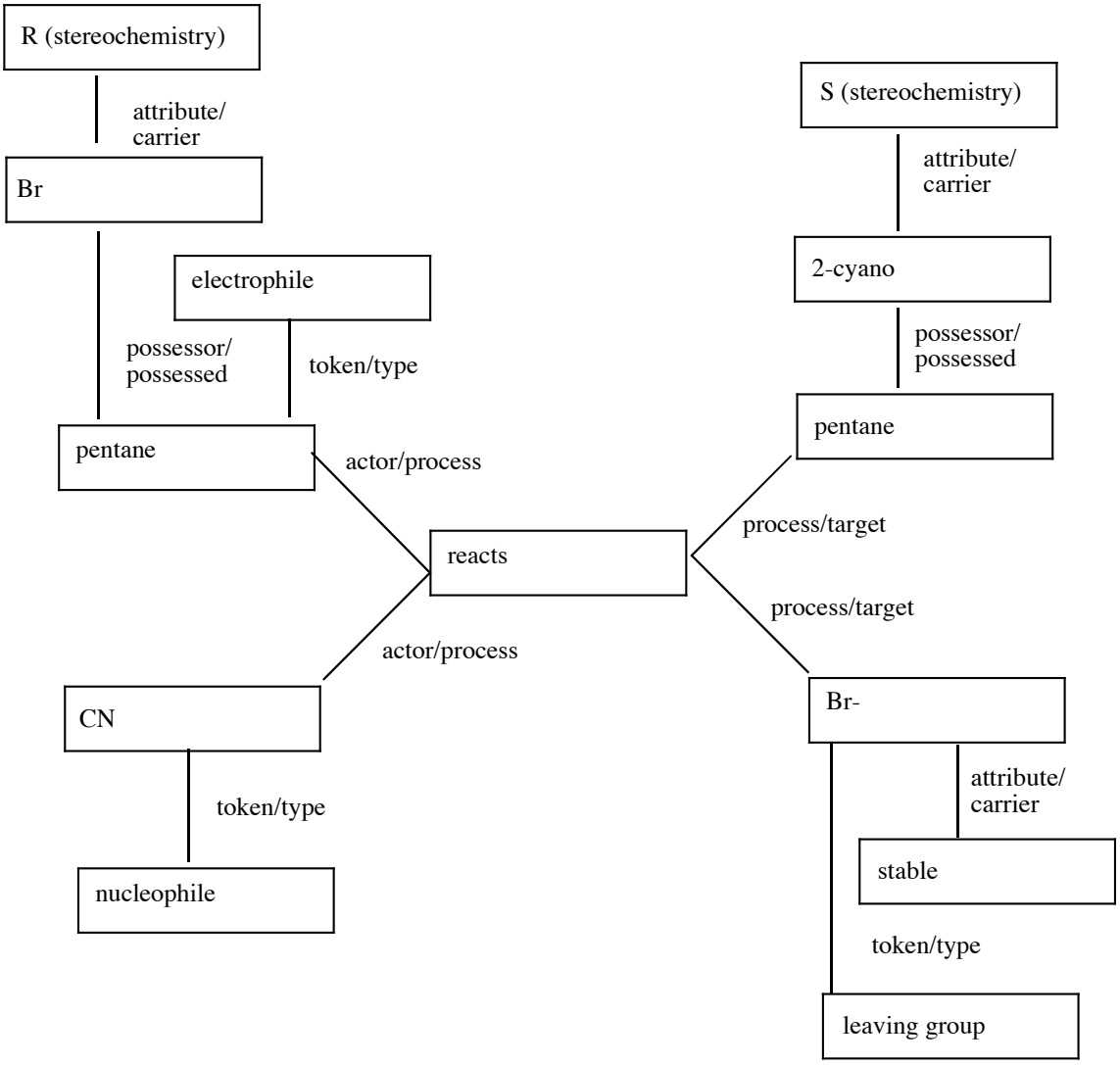


**Thematic Diagram for visual file wk8AdvYX**

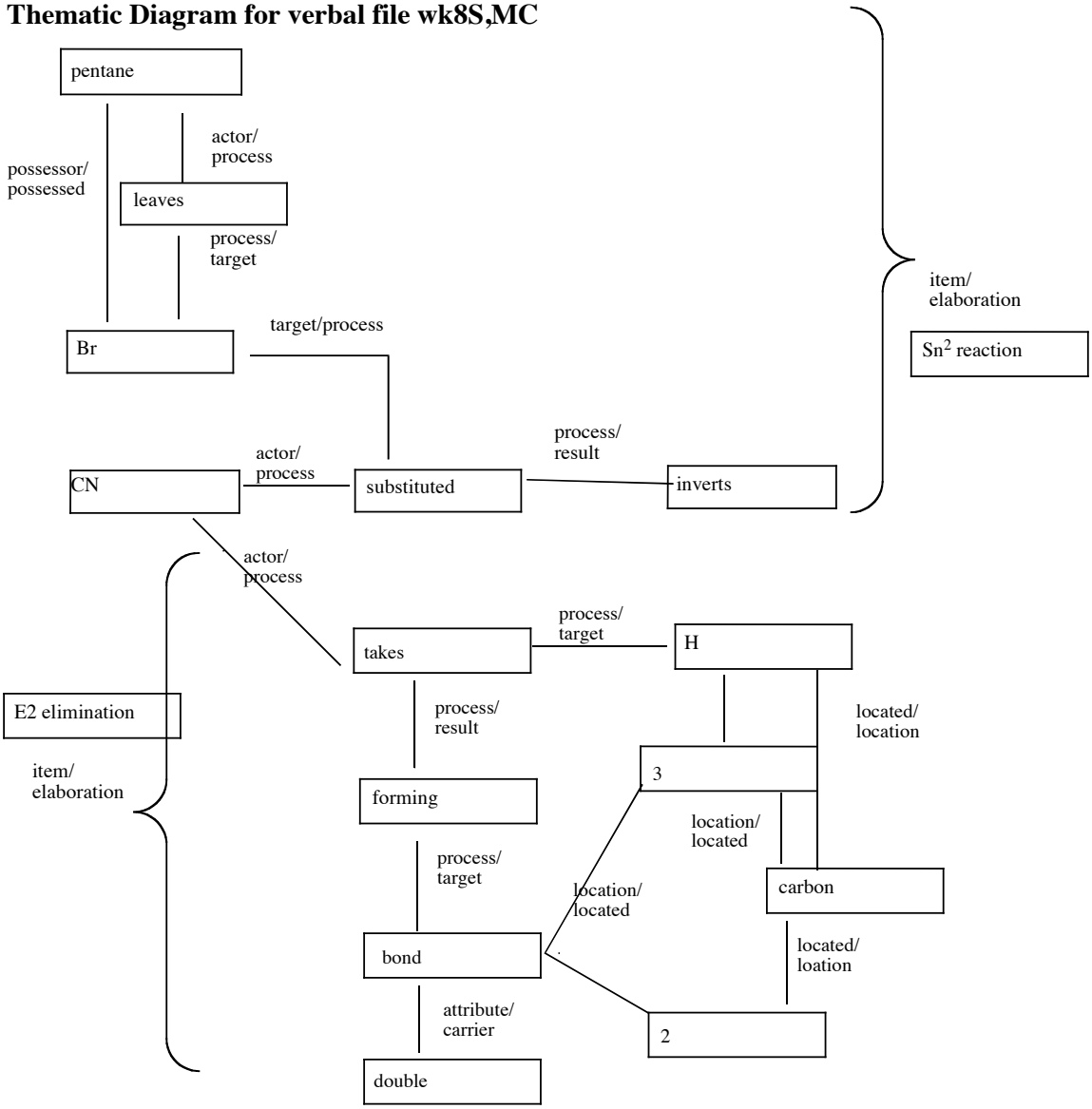


EGE (1999) PICTORIAL THEMATIC MAP

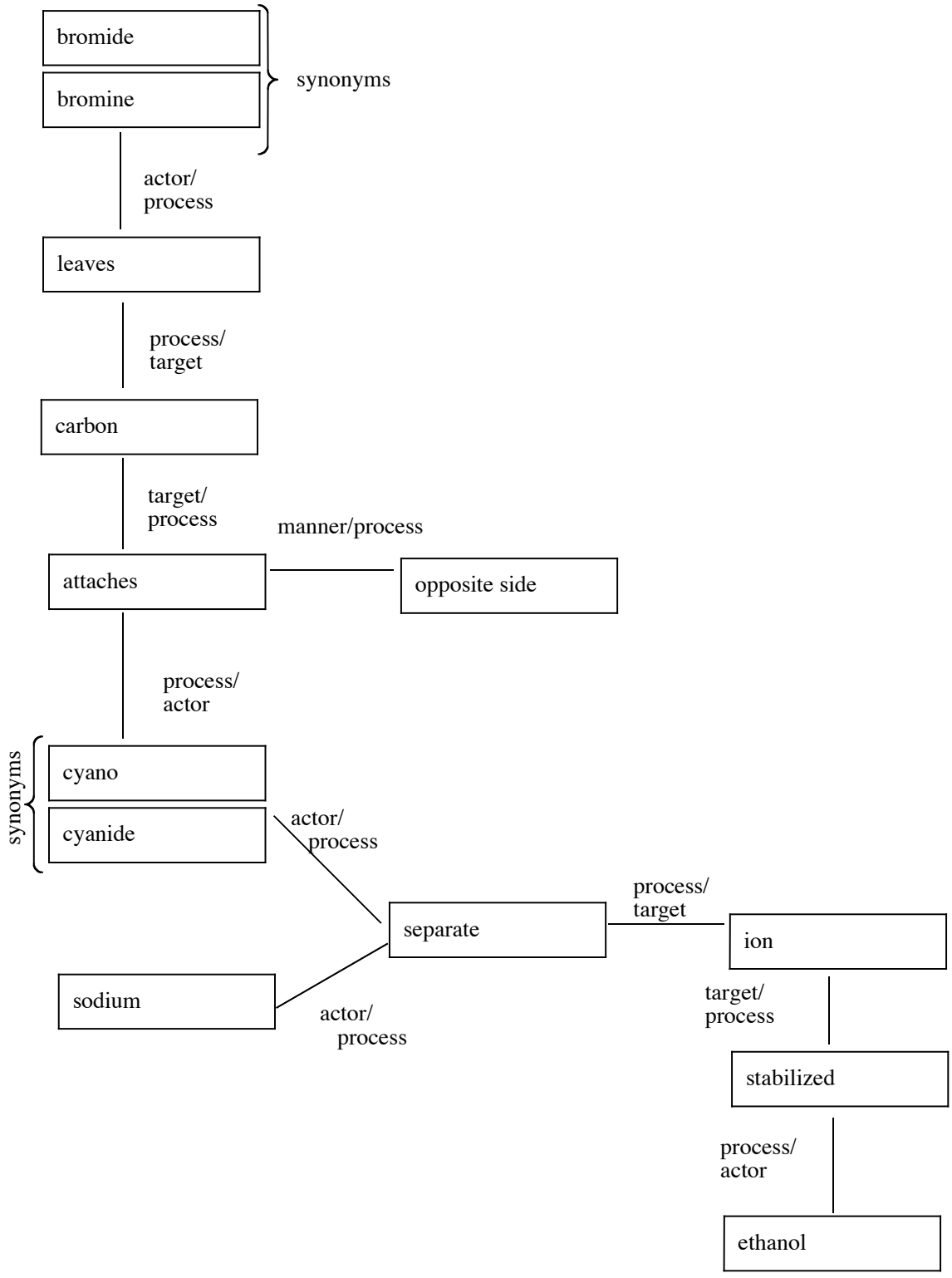
**Thematic Diagram from the textbook**



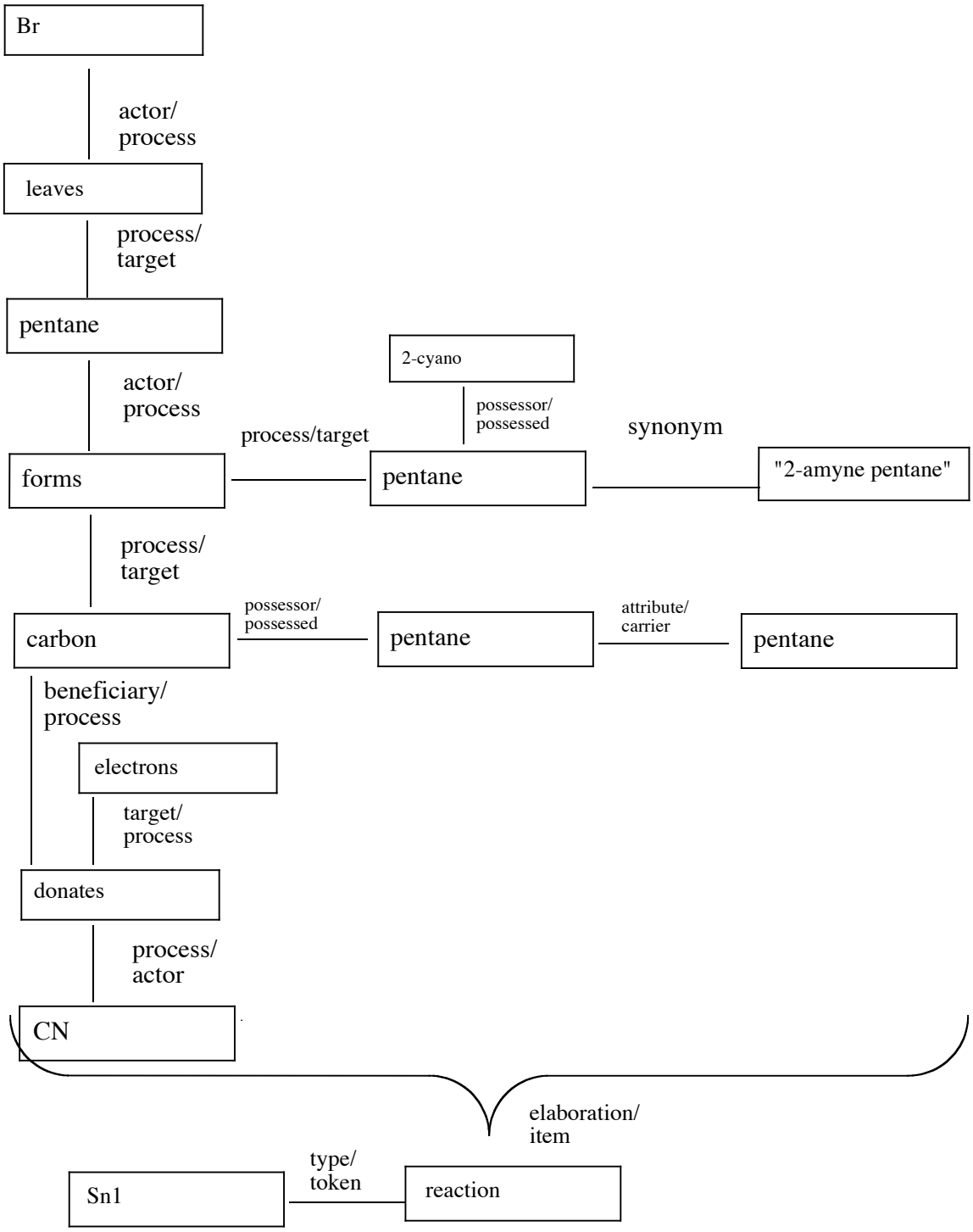
**Thematic Diagram for verbal file wk8S,MC**



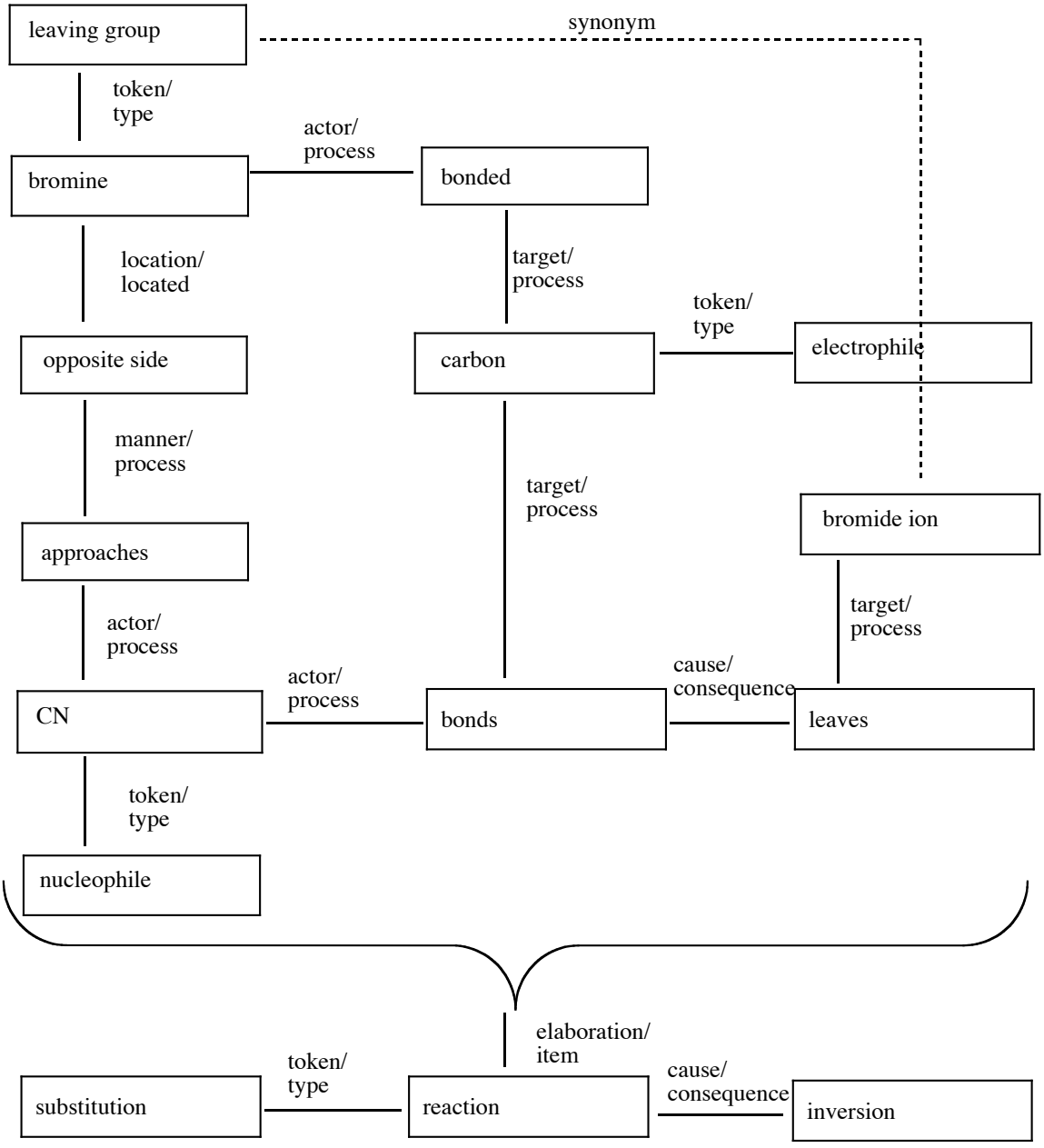
## Thematic Diagram for verbal file wk8Se,S



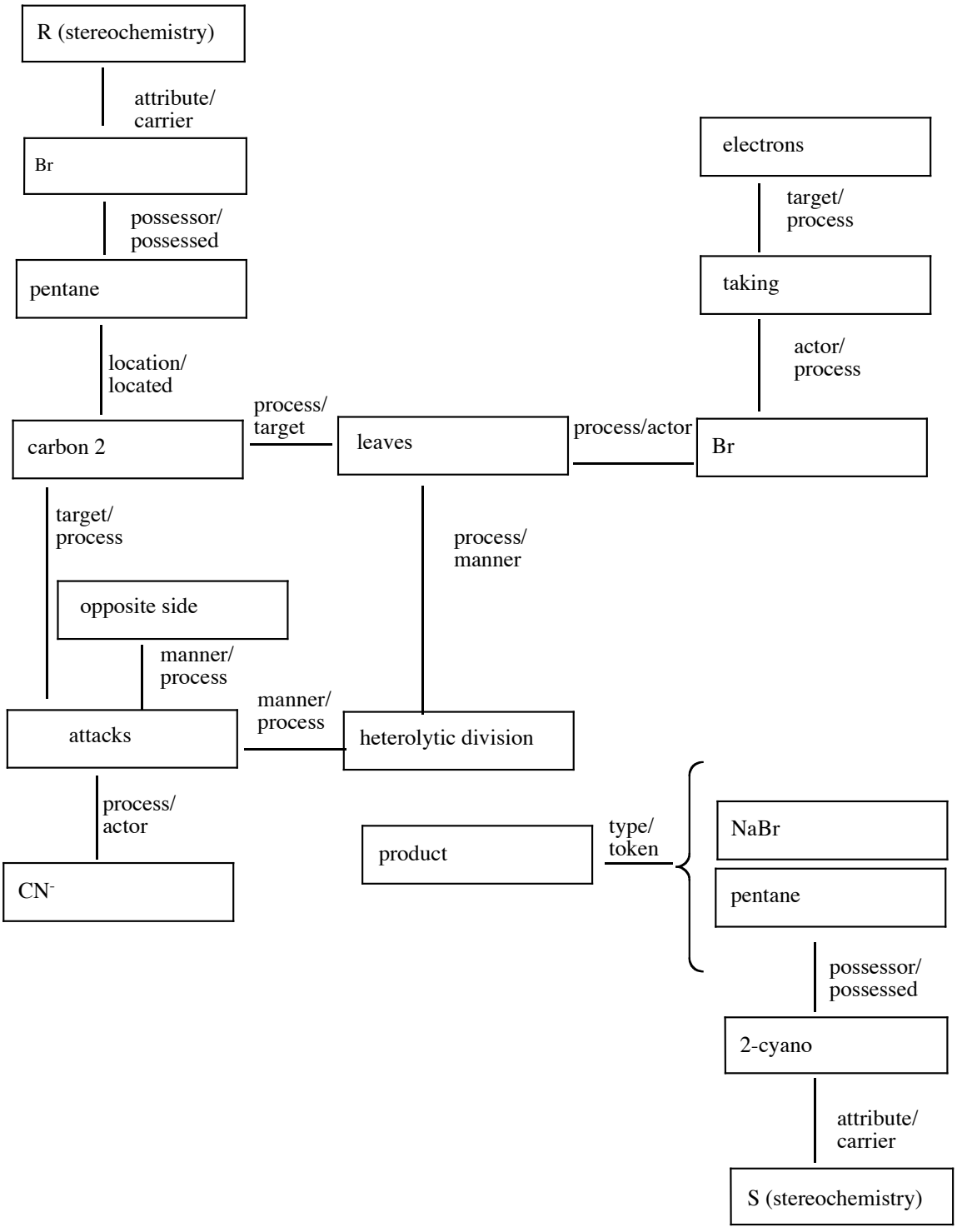
**Thematic Diagram for verbal file wk8N,AT**



**Thematic Diagram for verbal file wk8N,J**

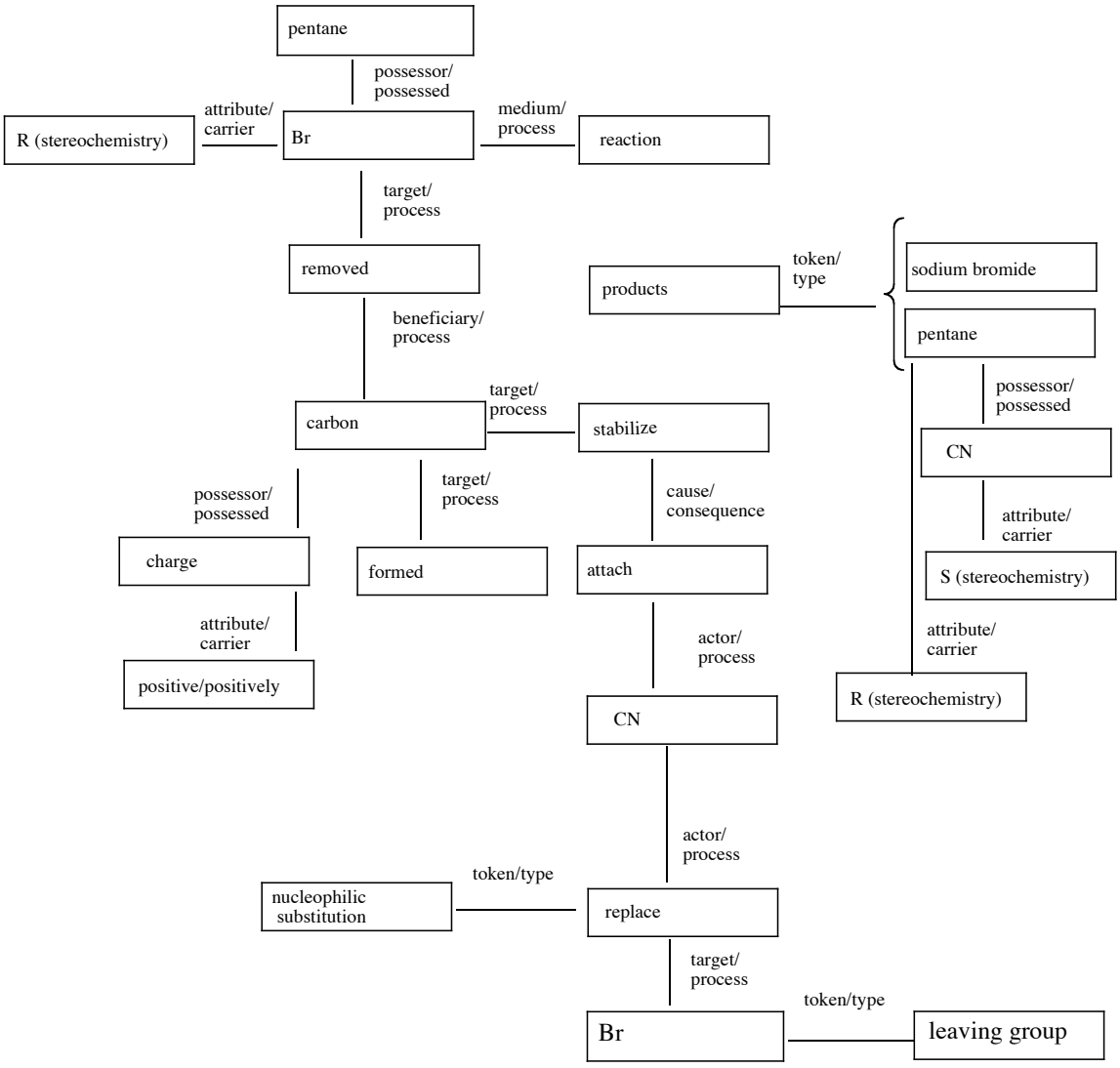


**Thematic Diagram for verbal file wk8N,JM**

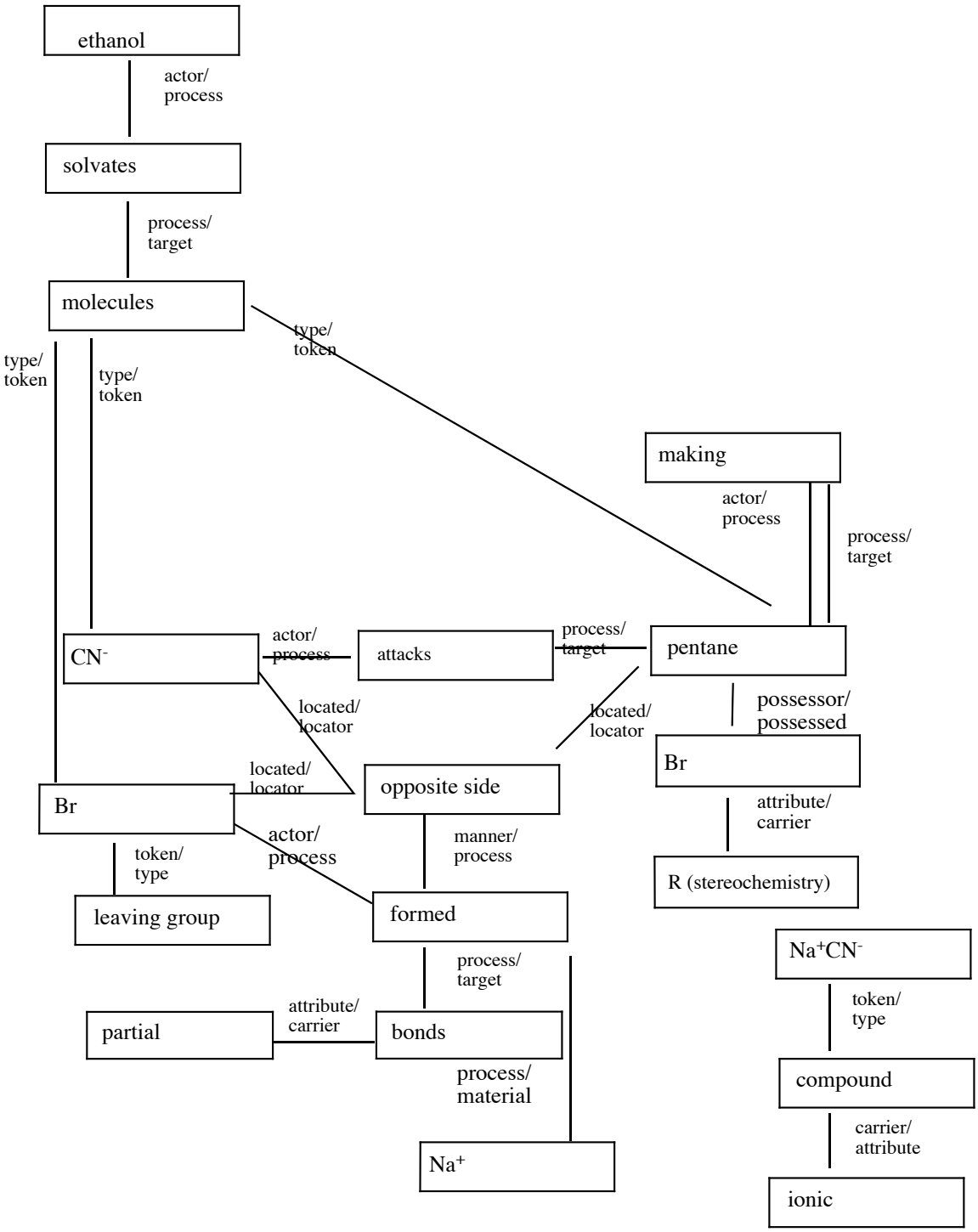


# TRADITIONAL GROUP VERBAL THEMATIC MAP

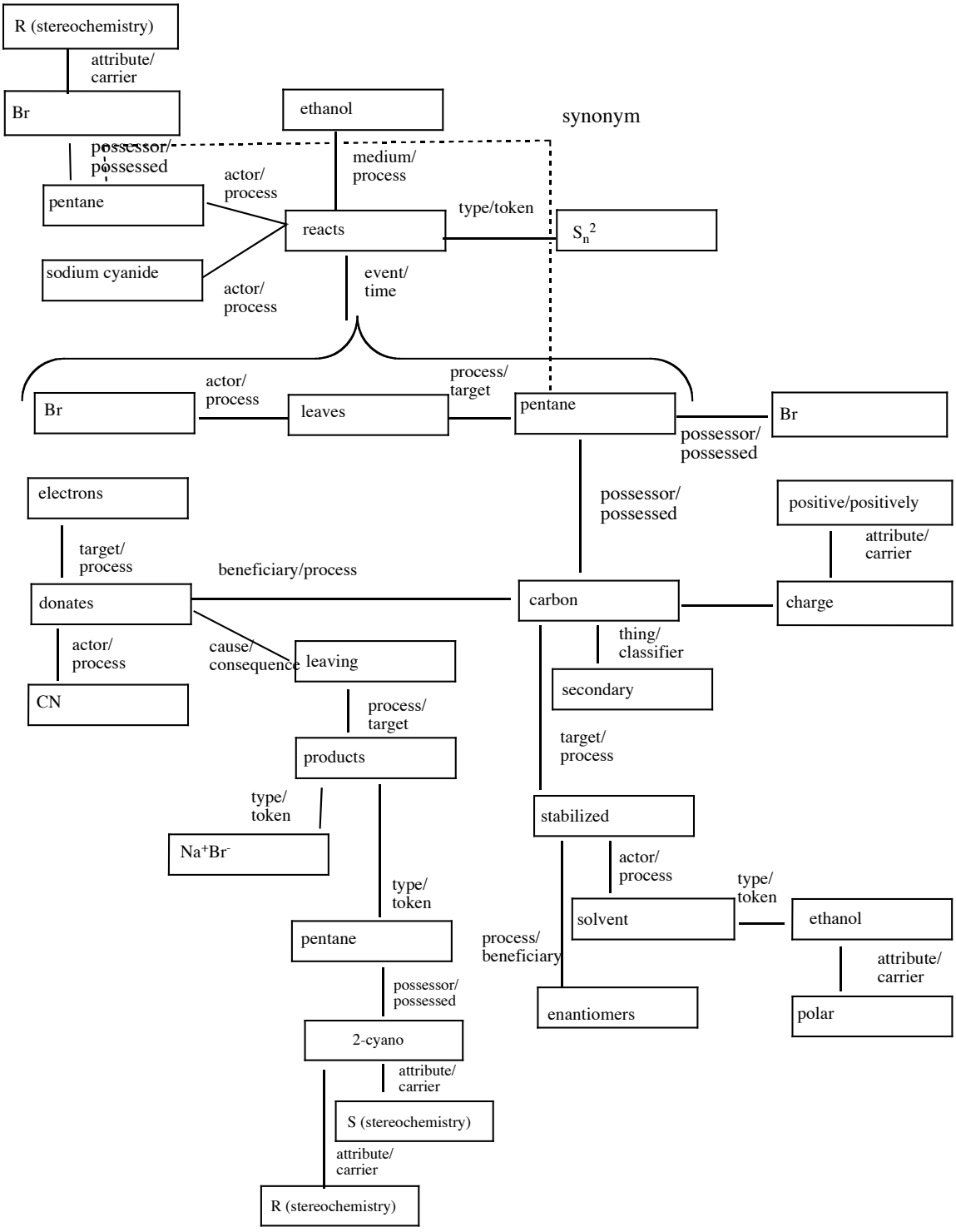
**Thematic Diagram for verbal file wk8AP,KZ**



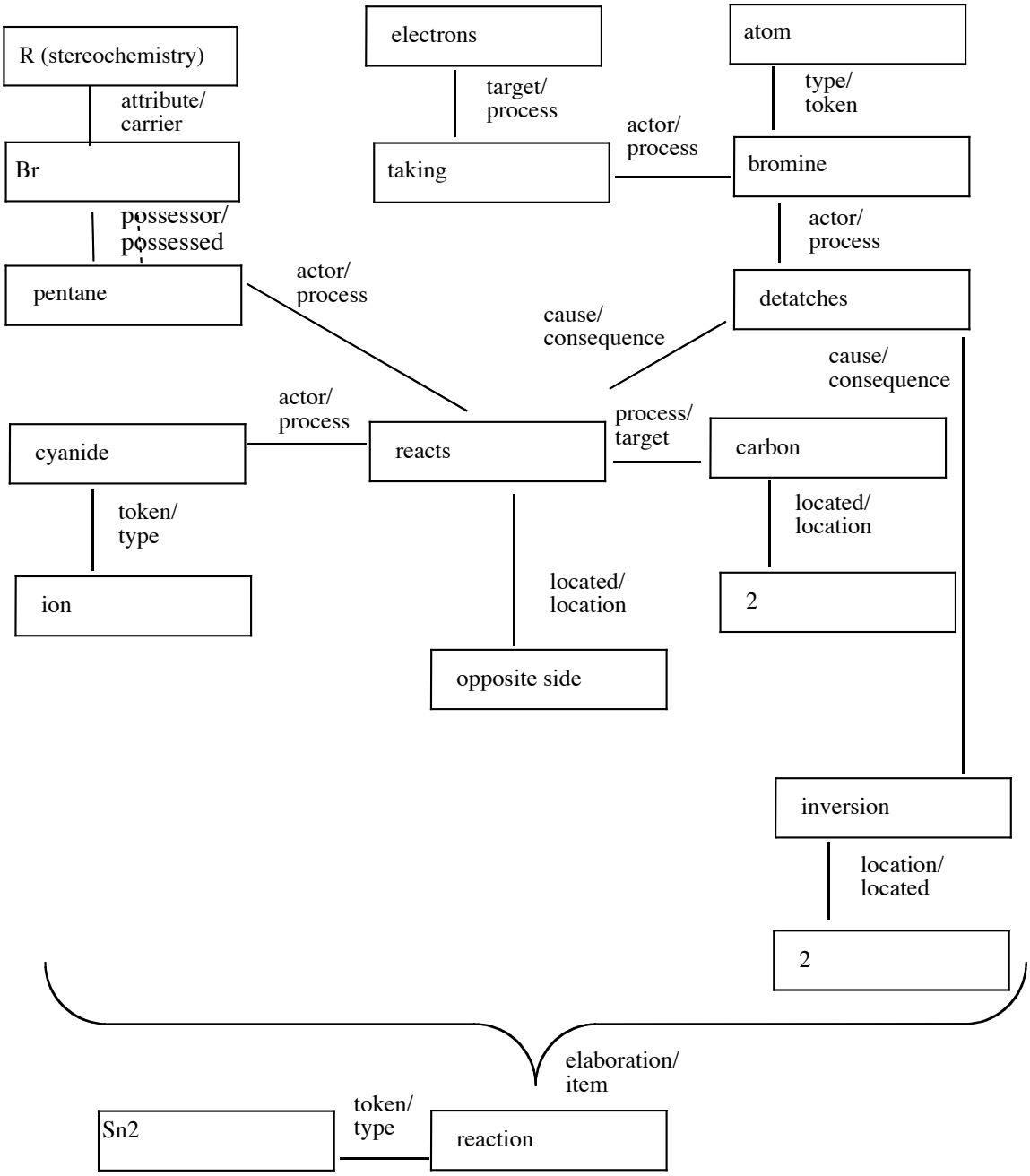
**Thematic Diagram for verbal file wk8CM,EF**



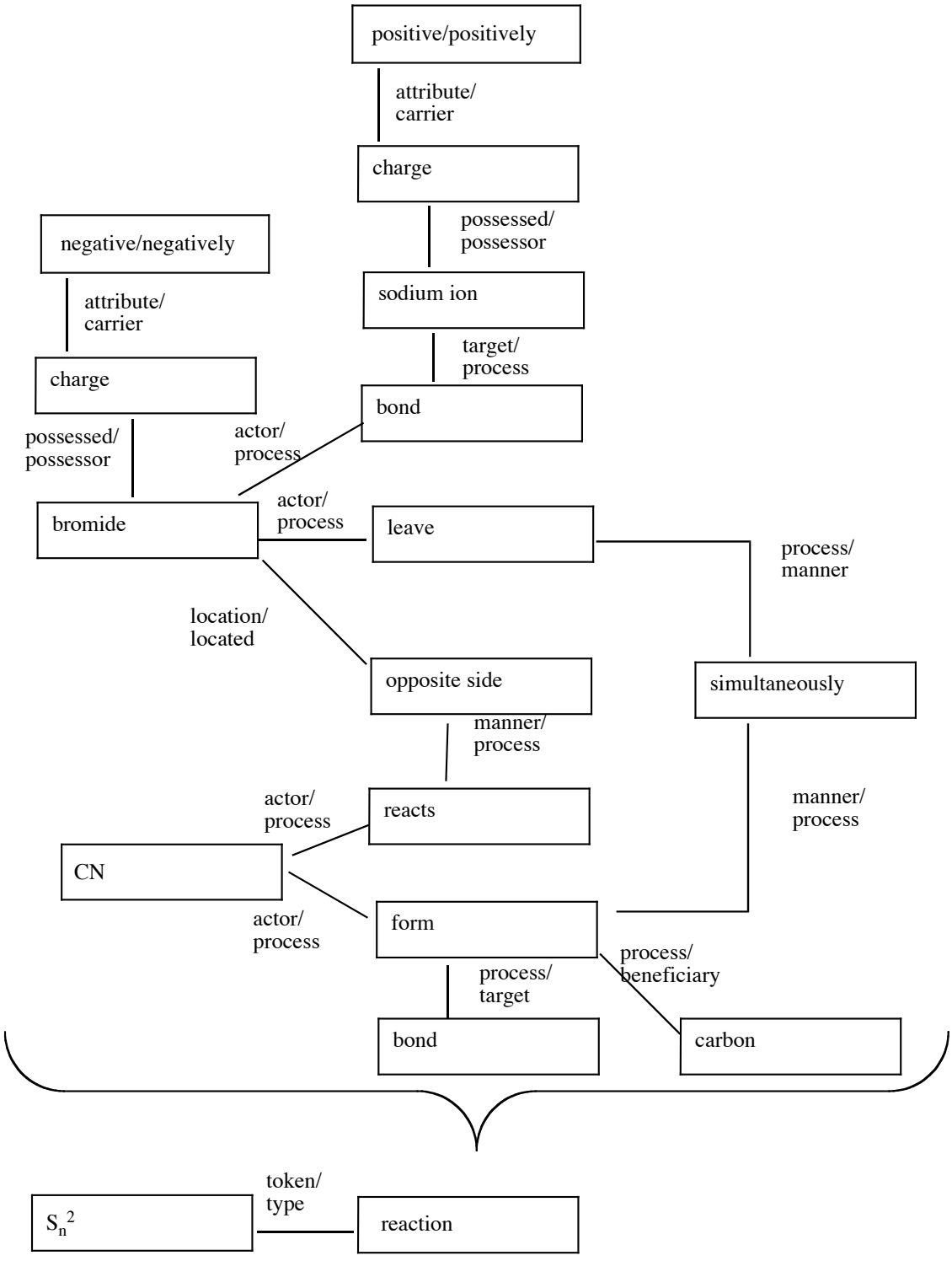
**Thematic Diagram for verbal file wk8CM,MP**



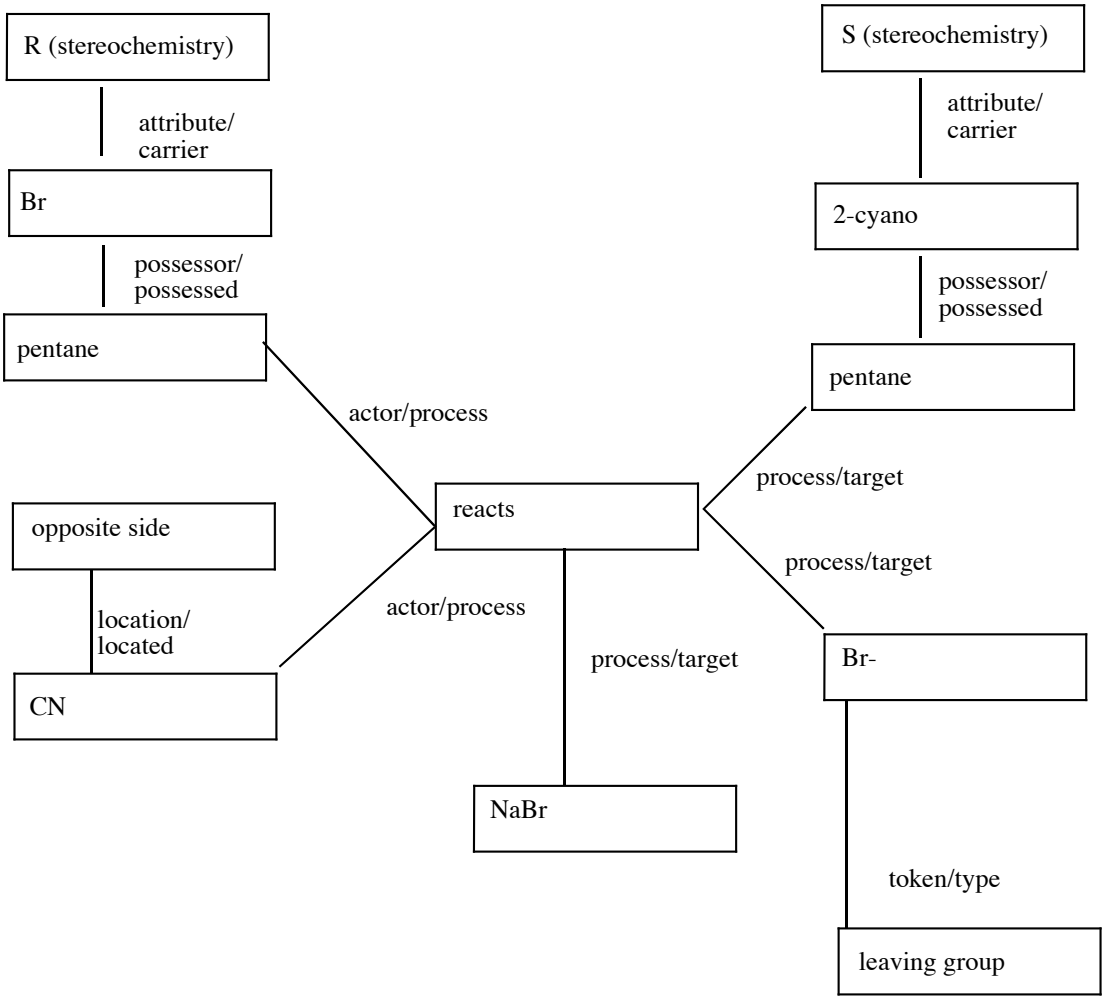
**Thematic Diagram for verbal file wk8DB,ES**



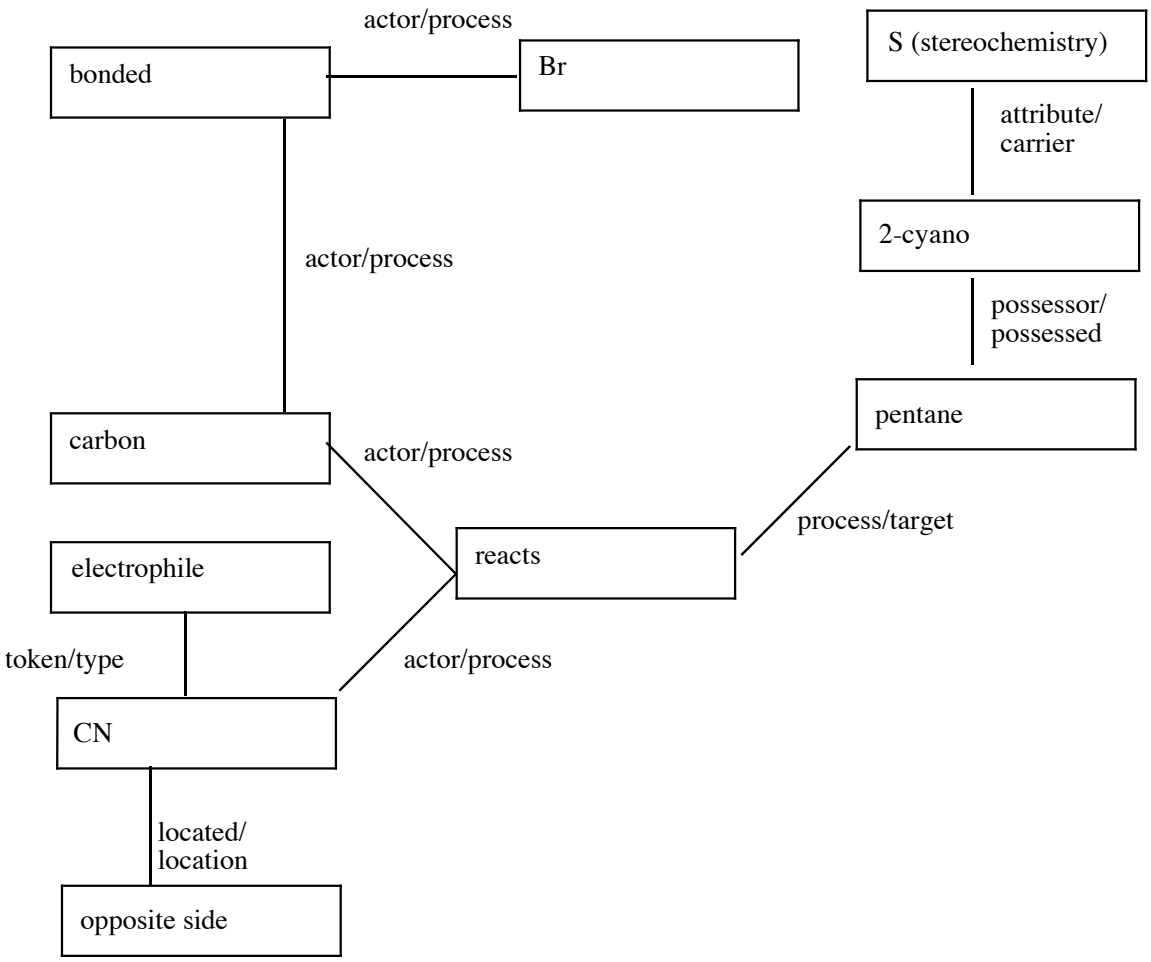
**Thematic Diagram for verbal file wk8DB,KK**



**Thematic Diagram for verbal file wk8AdvSR**



**Thematic Diagram for verbal file wk8AdvWG**



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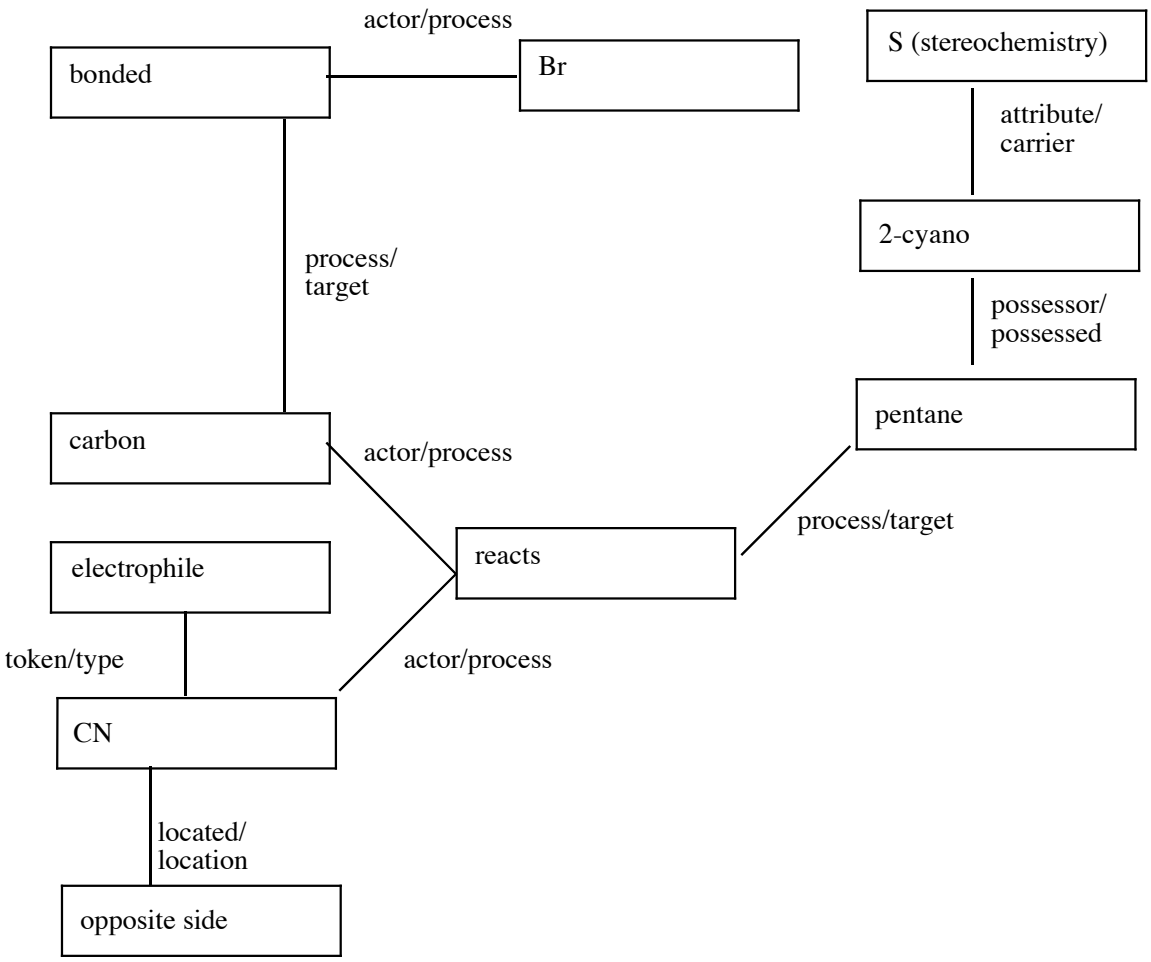
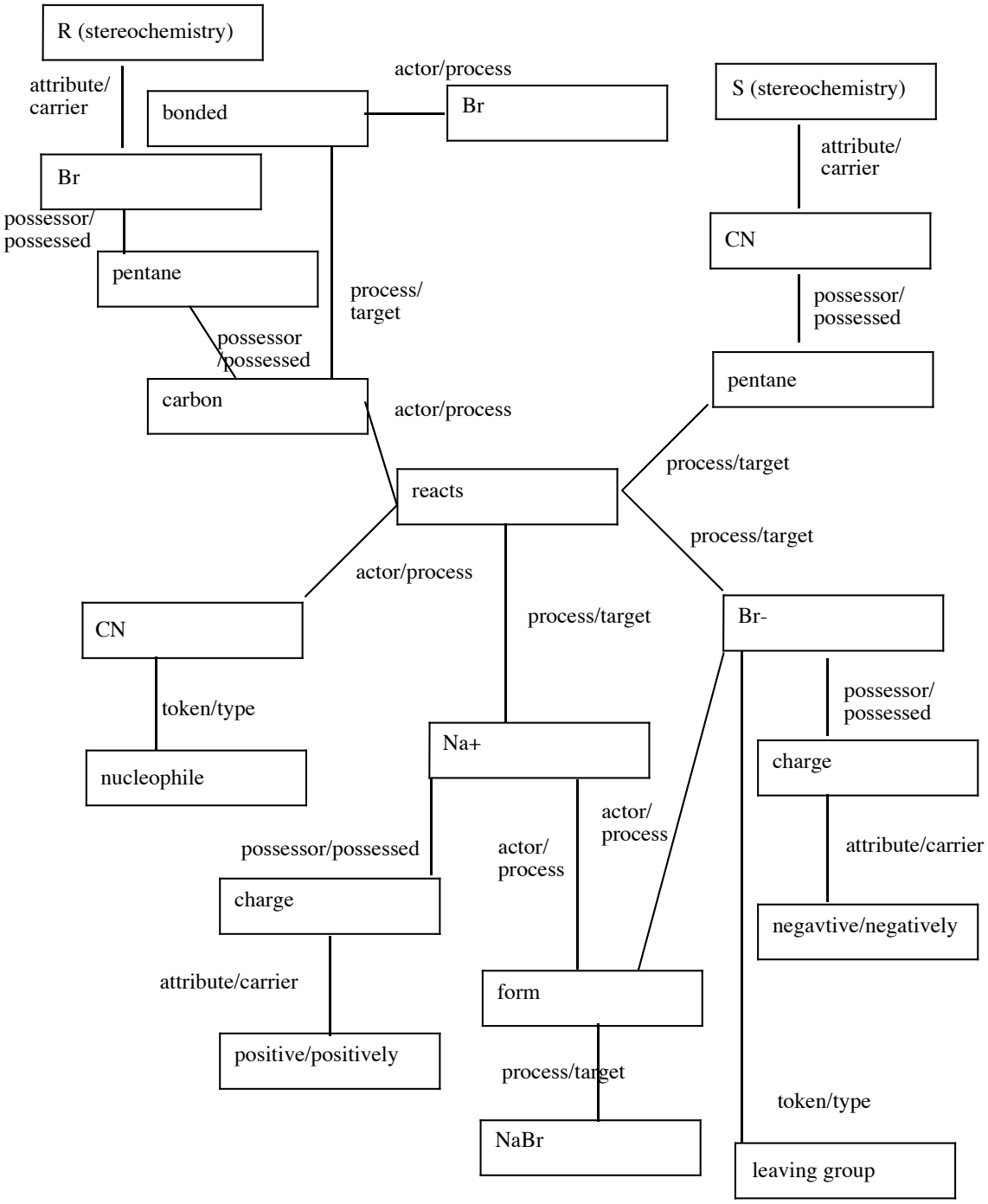
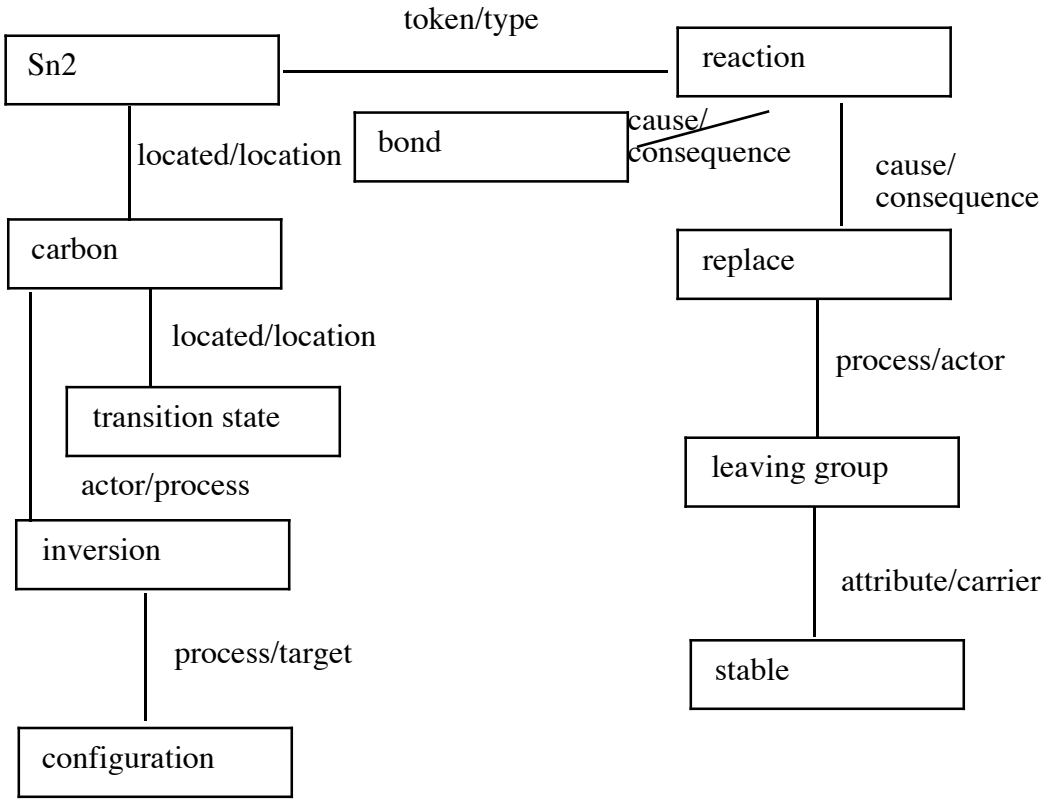


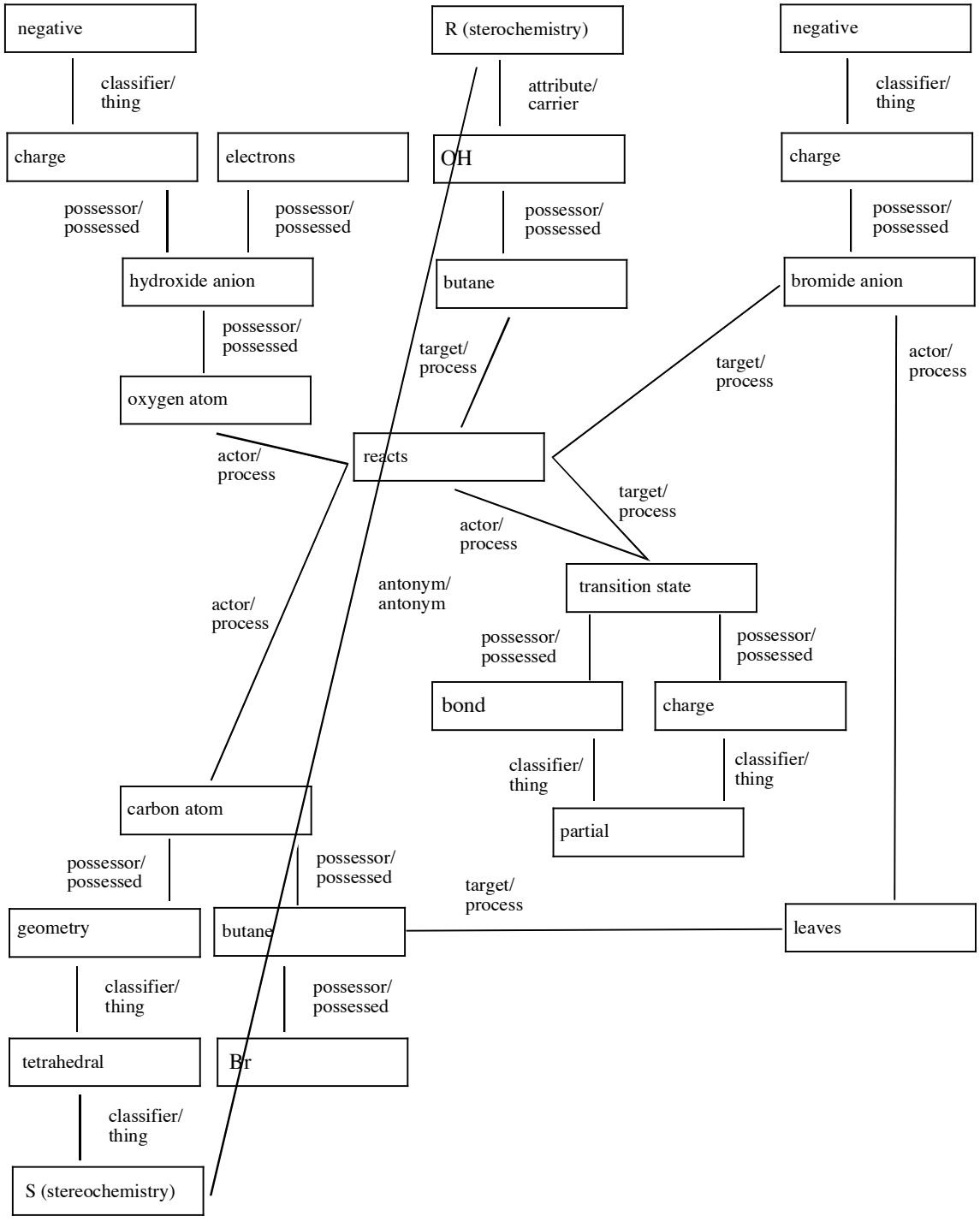
**Thematic Diagram for verbal file wk8AdvYX**



## Thematic Diagram for Textbook

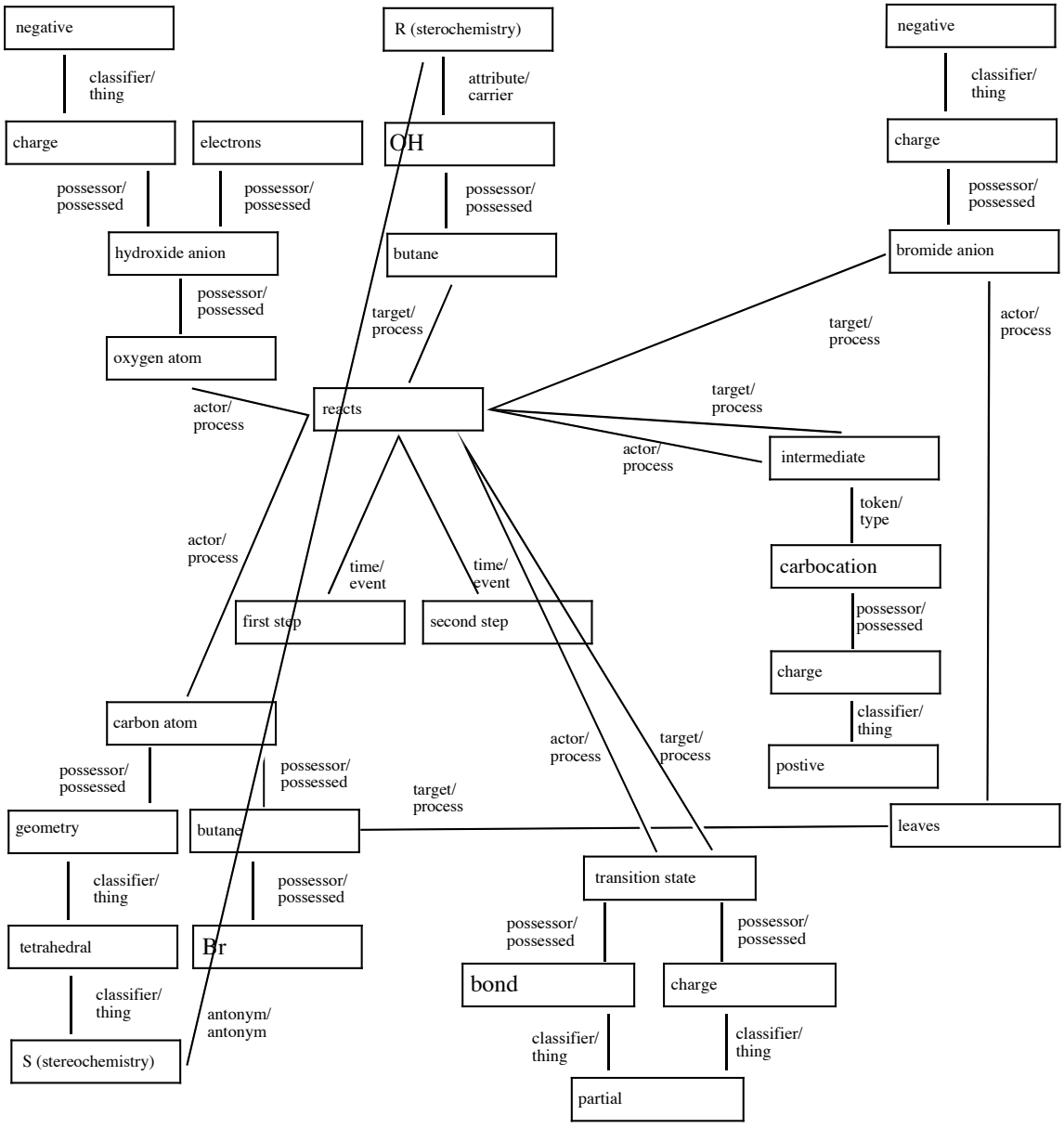


**Thematic Diagram for visual file McMurry SN2 (legend).jpg**



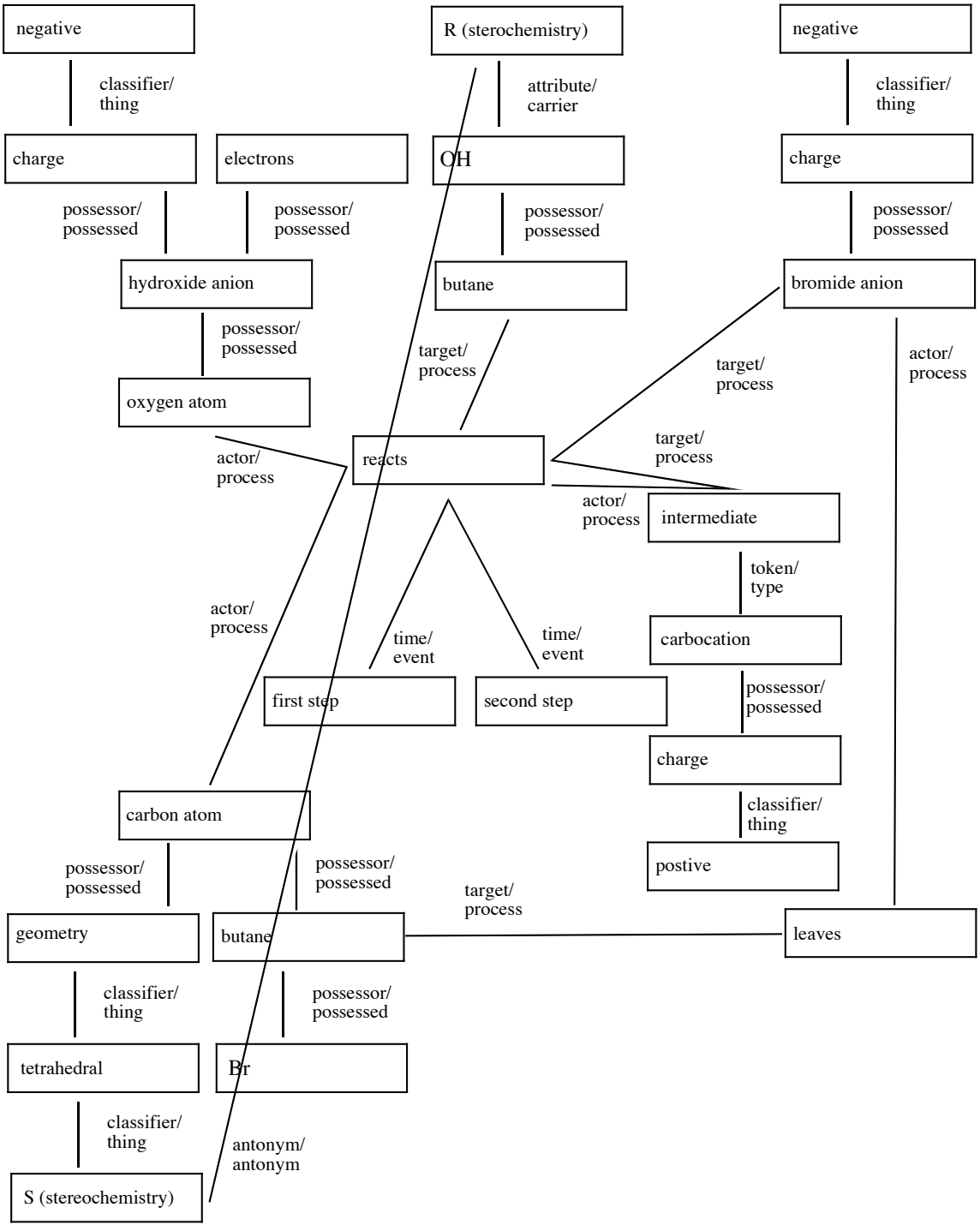
SN1-like inscription with transition state

**Thematic Diagram for visual file SN1-SN2mockups.cdx**



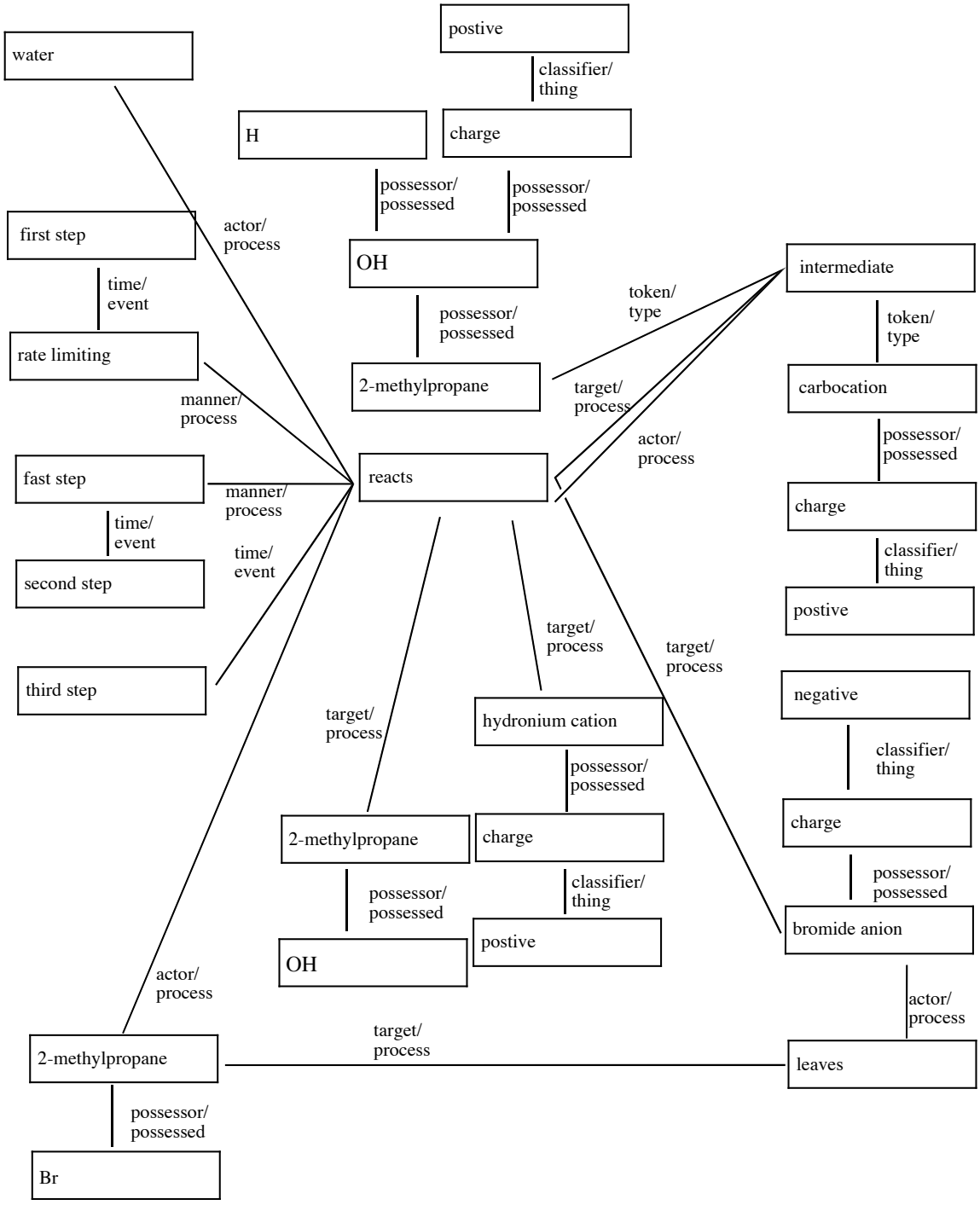
SN1-like inscription without transition state

**Thematic Diagram for visual file SN1-SN2mockups.cdx**

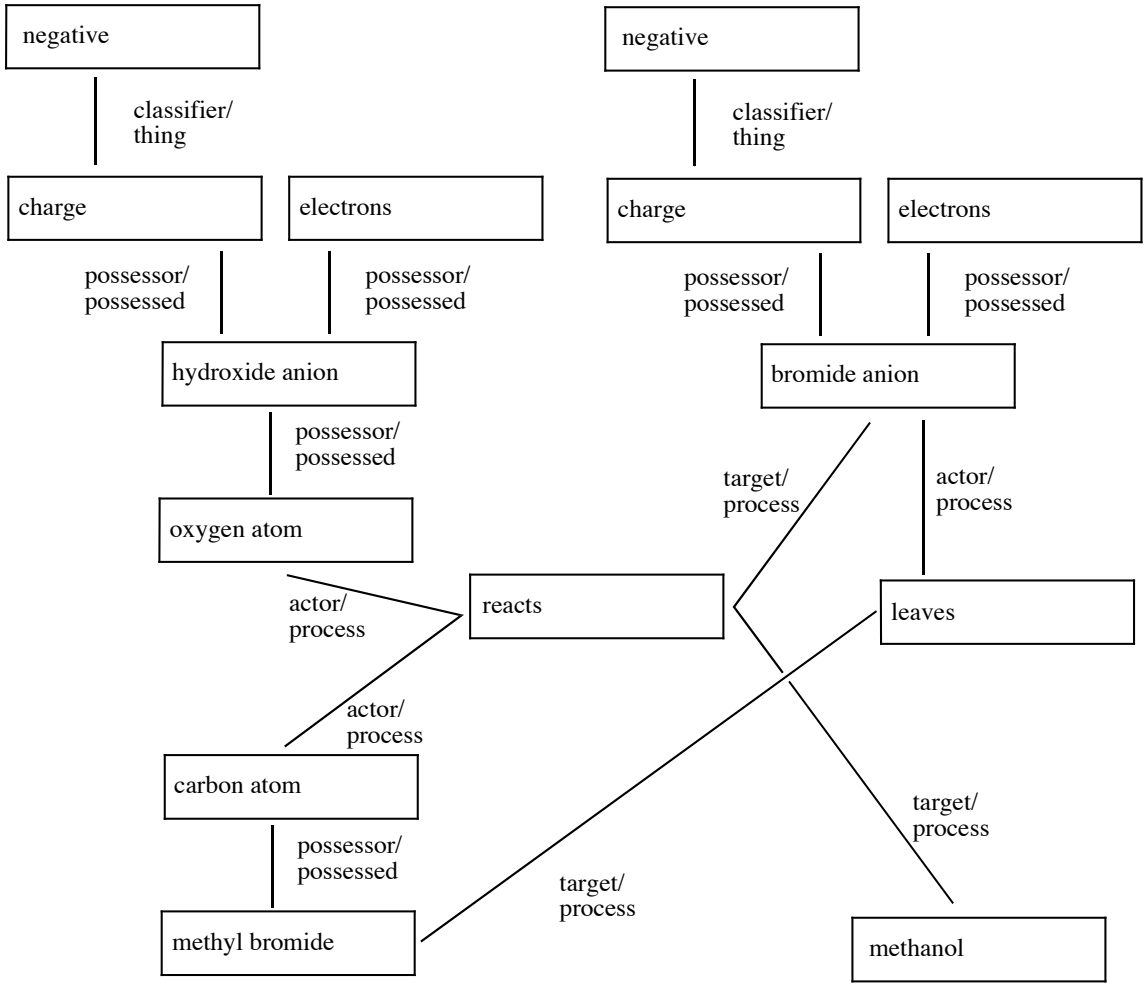


SN1 inscription

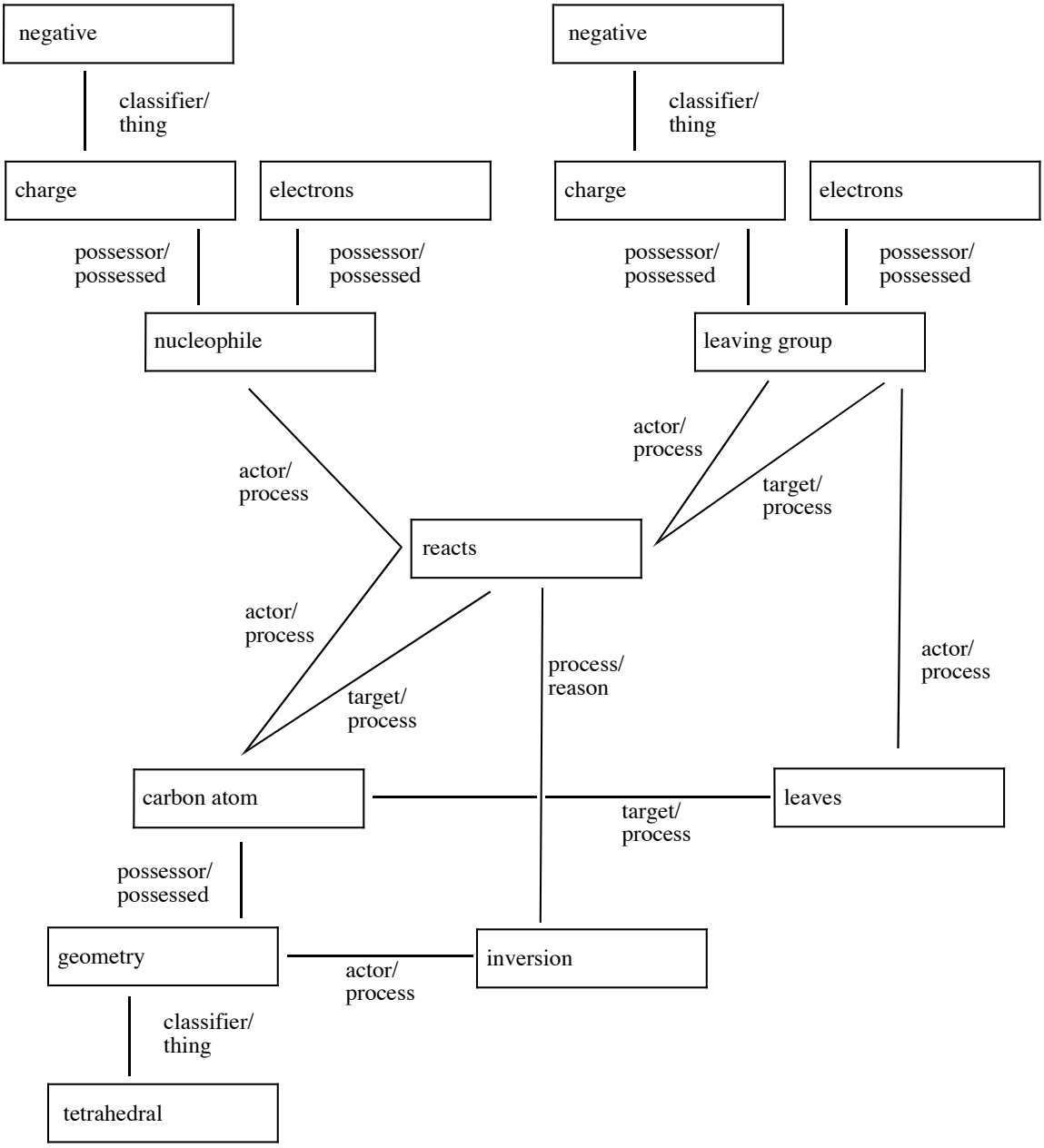
**Thematic Diagram for visual file AnalysisMcMurrySN1.doc**



**Thematic Diagram for visual file Bruice SN2.jpg**



**Thematic Diagram for visual file Fox SN2(all).jpg**

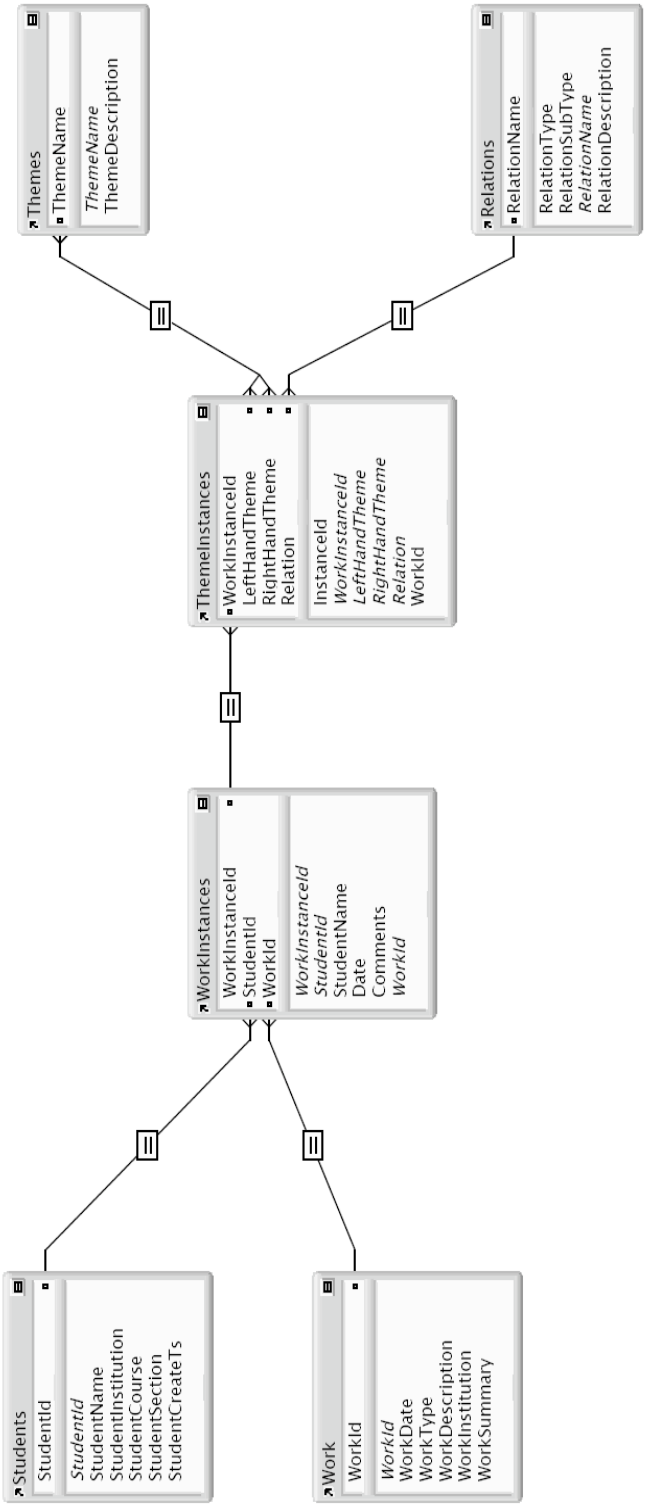


# APPENDIX C: DATABASE AND COMPARITOR DESCRIPTION

## DESCRIPTION OF DATABASE AND COMPARITOR TOOL

To facilitate analysis of student materials, we developed a database using FileMaker Developer 7.0. Once the student materials were coded and the data entered into the database, we exported the raw data to flat text files and performed similarity comparisons on that data using a small program written in the Perl 5 programming language. FileMaker is an inexpensive, commercial software product that runs on both MacOS and Windows platform computers. Perl 5 is a freely-available, open-source programming language that runs on most computing platforms and operating systems. The schema for the FileMaker database is shown in Figure 65.

**Figure 65. Schema for the FileMaker database.**



FILEMAKER DEVELOPER DATABASE DESIGN REPORT

The database definition and structure, including the description of all tables and fields, produced via the Filemaker "Database Design Report" utility, is shown in Table 42.

**Table 42. Database definition and structure.**

| Table Name | Statistics | Occurrences in Relationship Graph |
|---|---|---|
| Students | 6 fields defined, 22 records | *Students* |
| Themes | 2 fields defined, 113 records | *Themes* |
| Relations | 4 fields defined, 31 records | *Relations* |
| ThemeInstances | 6 fields defined, 1127 records | *ThemeInstances* |
| Work | 6 fields defined, 10 records | *Work* |
| WorkInstances | 6 fields defined, 63 records | *WorkInstances* |

Fields

**Table 43. Students - 6 fields**

| Field Name | Type | Options | Comments | In Relationships | In Value Lists |
|---|---|---|---|---|---|
| StudentId | Normal, Number | **Auto-Enter:**<br>Serial: Generate: On creation, Next value: 1029, Increment: 1<br>**Validation:**<br>Only during data entry<br>Strict validation<br>**Storage:**<br>Repetitions: 1<br>Indexing: All | Unique serial identifier for student record. | *Students=WorkInstances* | StudentList |
| StudentName | Normal, Text | **Validation:**<br>Always Validate<br>Not empty<br>Strict validation<br>**Storage:**<br>Repetitions: 1<br>Indexing: Minimal<br>Automatically create indexes as needed<br>Index Language: English | Full name of student (last,first). | | StudentList |
| StudentInstitution | Normal, Text | **Auto-Enter:**<br>Constant data: umich.edu<br>Allow editing<br>**Validation:** | Institution that this student belongs to. | | |

| | | | | | |
|---|---|---|---|---|---|
| | | Always Validate<br>Not empty<br>Strict validation<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | | | |
| StudentCourse | Normal, Text | **Validation:**<br>Always Validate<br>Not empty<br>Strict validation<br>Value list: CourseList<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | Identifier for course student is participating in. | | |
| StudentSection | Normal, Text | **Validation:**<br>Always Validate<br>Not empty<br>Strict validation<br>**Storage:**<br>Repetitions: 1 | Identifier for course section student is participating in. | | |

| | | | | | |
|---|---|---|---|---|---|
| | | Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | | | |
| StudentCreateTs | Normal, Timestamp | **Auto-Enter:**<br>Creation timestamp<br>**Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed | Timestamp student record was created. | | |



**Table 44. Themes - 2 Fields**

| Field Name | Type | Options | Comments | In Relationships | In Value Lists |
|---|---|---|---|---|---|
| ThemeName | Normal, Text | **Validation:**<br>Always Validate<br>Not empty<br>Strict validation<br>**Storage:**<br>Repetitions: 1<br>Indexing: Minimal<br>Automatically create indexes as needed | Name of theme. | *Themes∞ThemeInstances* | ThemeList |

| | | | | | |
|---|---|---|---|---|---|
| | | Index Language: English | | | |
| ThemeDescription | Normal, Text | **Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | Description of theme. | | |

**Table 45. Relations - 4 Fields**

| Field Name | Type | Options | Comments | In Relationships | In Value Lists |
|---|---|---|---|---|---|
| RelationType | Normal, Text | **Validation:**<br>Always Validate<br>Not empty<br>Strict validation<br>**Storage:**<br>Repetitions: 1<br>Indexing: Minimal<br>Automatically create indexes as needed<br>Index Language: English | Optional categorization for this relation. | | |
| RelationSubType | Normal, Text | **Validation:**<br>Always Validate<br>Not empty<br>Strict validation<br>**Storage:** | Optional sub-categorization for this relationship. | | |

| | | | | | |
|---|---|---|---|---|---|
| | | Repetitions: 1<br>Indexing: Minimal<br>Automatically create indexes as needed<br>Index Language: English | | | |
| RelationName | Normal, Text | **Validation:**<br>Always Validate<br>Not empty<br>Unique<br>Strict validation<br>**Storage:**<br>Repetitions: 1<br>Indexing: Minimal<br>Automatically create indexes as needed<br>Index Language: English | Name for this relationship. | *Relations=ThemeInstances* | RelationList |
| RelationDescription | Normal, Text | **Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | Description for this relationship. | | |



**Table 46. ThemeInstances - 6 Fields**

| Field Name | Type | Options | Comments | In Relationships | In Value Lists |
|---|---|---|---|---|---|
| InstanceId | Normal, | **Auto-Enter:**<br>Serial: Generate: On | Id for this thematic instance. | | |

| | | | | | |
|---|---|---|---|---|---|
| | Number | creation, Next value: 2164, Increment: 1<br>**Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: All | | | |
| WorkInstanceId | Normal, Number | **Validation:**<br>Only during data entry<br>Value list: WorkInstanceList<br>**Storage:**<br>Repetitions: 1<br>Indexing: All | Id of WorkInstance that this theme was used in. | *WorkInstances=ThemeInstances* | |
| LeftHandTheme | Normal, Text | **Validation:**<br>Only during data entry<br>Value list: ThemeList<br>**Storage:**<br>Repetitions: 1<br>Indexing: Minimal<br>Automatically create indexes as needed<br>Index Language: English | Left-hand theme used. | *Themes∞ThemeInstances* | |
| RightHandTheme | Normal, Text | **Validation:**<br>Only during data entry<br>Value list: ThemeList<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create | Right-hand Theme used. | *Themes∞ThemeInstances* | |

| | | | | | |
|---|---|---|---|---|---|
| | | indexes as needed<br>Index Language: English | | | |
| Relation | Normal, Text | **Validation:**<br>Only during data entry<br>Value list: RelationList<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | Relation used. | *Relations=ThemeInstances* | |
| WorkId | Normal, Number | **Auto-Enter:**<br>Lookup: *WorkInstances* ::WorkId , Do not copy, Don't copy contents if empty<br>**Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed | Id of Work that this theme was used in. | | |



**Table 47. Work - 6 Fields**

| Field Name | Type | Options | Comments | In Relationships | In Value Lists |
|---|---|---|---|---|---|
| WorkId | Normal, Numb | **Auto-Enter:**<br>Serial: Generate: On creation, Next value: 20, | Identifier for work unit (assignment, test, etc.) | *Work=WorkInstances* | WorkList |

| | | | | | |
|---|---|---|---|---|---|
| | er | Increment: 1<br>**Validation:**<br>Always Validate<br>Strict validation<br>**Storage:**<br>Repetitions: 1<br>Indexing: All | | | |
| WorkDate | Normal, Date | **Auto-Enter:**<br>Creation date<br>Allow editing<br>**Validation:**<br>Only during data entry<br>Strict data type: 4 digit year<br>Error message: Lets use four year dates just to avoid issues.<br>**Storage:**<br>Repetitions: 1<br>Indexing: All | Date that the work was performed. | | |
| WorkType | Normal, Text | **Validation:**<br>Only during data entry<br>Value list: WorkTypeList<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | Exam, assignment, etc. | | |

| | | | | | |
|---|---|---|---|---|---|
| WorkDescription | Normal, Text | **Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | Description of this work. | | |
| WorkInstitution | Normal, Text | **Auto-Enter:**<br>Constant data: umich.edu<br>Allow editing<br>**Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | Institution associated with this work. | | |
| WorkSummary | Calculated, Text | **Calculation:**<br>*Work* ::WorkDate & " " & *Work* ::WorkType & " " & *Work* ::WorkInstitution<br>**Storage:**<br>Repetitions: 1<br>Indexing: All<br>Index Language: English | Auto-generated field combining work date, work type, and work institution. Useful for reports. | | WorkList |

**Table 48. WorkInstances - 6 Fields**

| Field Name | Type | Options | Comments | In Relationships | In Value Lists |
|---|---|---|---|---|---|
| WorkInstanceId | Normal, Number | **Auto-Enter:**<br>Serial: Generate: On creation, Next value: 1079, Increment: 1<br>**Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: All | Unique identifier for this work instance. | *WorkInstances=ThemeInstances* | |
| StudentId | Normal, Number | **Validation:**<br>Only during data entry<br>Value list: StudentList<br>**Storage:**<br>Repetitions: 1<br>Indexing: All | Unique identifier for the student associated with this work instance. | *Students=WorkInstances* | |
| StudentName | Normal, Text | **Auto-Enter:**<br>Lookup: *Students* ::StudentName , Do not copy, Don't copy contents if empty<br>**Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | | | |

| | | | | | |
|---|---|---|---|---|---|
| Date | Normal, Date | **Auto-Enter:**<br>Creation date<br>Allow editing<br>**Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed | Date associated with this work instance. | | |
| Comments | Normal, Text | **Validation:**<br>Only during data entry<br>**Storage:**<br>Repetitions: 1<br>Indexing: None<br>Automatically create indexes as needed<br>Index Language: English | Optional comments. | | |
| WorkId | Normal, Number | **Validation:**<br>Only during data entry<br>Strict validation<br>Value list: WorkList<br>**Storage:**<br>Repetitions: 1<br>Indexing: All | Unique identifer for the work this is an instance of. | *Work=WorkInstances* | |

**Table 49. Relationships: Table Occurrences**

| Table Occurrence | Source Table | In Relationships | In Field Definitions | In Value Lists | Associated with layouts |
|---|---|---|---|---|---|
| *Relations* | Relations | *Relations=ThemeInstances* | | RelationList | Relations |
| *Themes* | Themes | *Themes∞ThemeInstances* | | ThemeList | Themes |
| *Work* | Work | *Work=WorkInstances* | *Work* ::WorkSummary | WorkList | Work Data Entry<br>Work |
| *Students* | Students | *Students=WorkInstances* | *WorkInstances* ::StudentName | StudentList | Students |
| *ThemeInstances* | ThemeInstances | *WorkInstances=ThemeInstances*<br>*Themes∞ThemeInstances*<br>*Relations=ThemeInstances* | | | WorkInstance Data Entry<br>ThemeInstances |
| *WorkInstances* | WorkInstances | *Work=WorkInstances*<br>*Students=WorkInstances*<br>*WorkInstances=ThemeInstances* | *ThemeInstances* ::WorkId | WorkInstanceList | Work Data Entry<br>WorkInstance Data Entry |



**Table 50. Relationship: *Work=WorkInstances***

| Table Occurrence | *Work* | | *WorkInstances* |
|---|---|---|---|
| **Field** | WorkId | = | WorkId |
| **Source Table** | Work | | WorkInstances |
| **Allow creation of records via this relationship** | Off | | On |
| **Delete related** | Off | | Off |

| | | | |
|---|---|---|---|
| **records in this table when a record is deleted in the other table** | | | |
| **Sort records** | Off | | Off |

**Table 51. Relationship: Students=WorkInstances**

| **Table Occurrence** | *Students* | | *WorkInstances* |
|---|---|---|---|
| **Field** | StudentId | = | StudentId |
| **Source Table** | Students | | WorkInstances |
| **Allow creation of records via this relationship** | Off | | Off |
| **Delete related records in this table when a record is deleted in the other table** | Off | | Off |
| **Sort records** | Off | | Off |



**Table 52. Relationship: *WorkInstances=ThemeInstances***

| **Table Occurrence** | *WorkInstances* | | *ThemeInstances* |
|---|---|---|---|

| | | | |
|---|---|---|---|
| **Field** | WorkInstanceId | = | WorkInstanceId |
| **Source Table** | WorkInstances | | ThemeInstances |
| **Allow creation of records via this relationship** | Off | | On |
| **Delete related records in this table when a record is deleted in the other table** | Off | | Off |
| **Sort records** | Off | | Off |

**Table 53. Relationship: *Themes=ThemeInstances***

| **Table Occurrence** | *Themes* | | *ThemeInstances* |
|---|---|---|---|
| **Field** | ThemeName | = | LeftHandTheme |
| **and** | ThemeName | = | RightHandTheme |
| **Source Table** | Themes | | ThemeInstances |
| **Allow creation of records via this relationship** | Off | | Off |
| **Delete related records in this table when a record is deleted in the other table** | Off | | Off |
| **Sort records** | Off | | Off |

**Table 54. Relationship: *Relations=ThemeInstances***

| **Table Occurrence** | *Relations* | | *ThemeInstances* |
|---|---|---|---|
| **Field** | RelationName | = | Relation |
| **Source Table** | Relations | | ThemeInstances |
| **Allow creation of records via this relationship** | Off | | Off |
| **Delete related records in this table when a record is deleted in the other table** | Off | | Off |
| **Sort records** | Off | | Off |

## "COMPARATOR" DATA ANALYSIS PROGRAM

The data analysis program, called "comparator.pl" was written in Perl 5, a freely-available open-source programming language available on all common computing platforms. The purpose of the program is to enable comparison of student works (i.e. each particular student's completion of an assignment, exam, etc.) in terms of the number of Theme-Relation-Theme triplets they have in common, and thus their similarity.

Perl 5 uses an encapsulation and extension mechanism called "modules." In addition to the modules included in the standard Perl distribution, comparator.pl uses version 1.20 of the Set::Scalar module to perform set comparisons. The functionality of the Set::Scalar module was verified by running the standard test harness that comes with the module. The overall proper functioning of the comparator.pl program was verified by comparing its output to manual computations.

Comparator.pl was coded using a simple text editor. No other special tools were required. The source code for the comparator.pl program is as follows:

```
#!/usr/bin/perl

use Set::Scalar;
use Getopt::Long;
use Tie::File;
use Fcntl 'O_RDONLY';
#use strict;

$VERSION = '0.4.3';

#Getopt::Long::Configure("debug");

# Set defaults for options.
my $DEFAULT_DATA_DIR = '.';
my $DEFAULT_FILE_STUDENTS = 'students.tab';
my $DEFAULT_FILE_WORK = 'work.tab';
my $DEFAULT_FILE_WORKINSTANCES = 'workinstances.tab';
my $DEFAULT_FILE_THEMEINSTANCES = 'themeinstances.tab';
my $DEFAULT_SEPARATOR_CHAR = ':';
```

```
my $DEFAULT_VERBOSE = 0;
my $DEFAULT_PRECISION = 4;

my $DATA_DIR = $DEFAULT_DATA_DIR;
my $FILE_STUDENTS = $DEFAULT_FILE_STUDENTS;
my $FILE_WORK = $DEFAULT_FILE_WORK;
my $FILE_WORKINSTANCES = $DEFAULT_FILE_WORKINSTANCES;
my $FILE_THEMEINSTANCES = $DEFAULT_FILE_THEMEINSTANCES;
my $SEPARATOR_CHAR = $DEFAULT_SEPARATOR_CHAR;
my $VERBOSE = $DEFAULT_VERBOSE;
my $PRECISION = $DEFAULT_PRECISION;

sub usage {
      print "Usage: $0 [options] <workinstanceid1> <workinstanceid2>
...\n";
    print "       $0 -h | --help (to show all options)\n\n";
}
usage() unless (@ARGV);

$usagestatus = GetOptions (
      "datadir=s" => \$DATA_DIR,
      "studentsfile=s" => \$FILE_STUDENTS,
      "workfile=s" => \$FILE_WORK,
      "workinstancesfile=s" => \$FILE_WORKINSTANCES,
      "themeinstancesfile=s" => \$FILE_THEMEINSTANCES,
      "verbose|v" => \$VERBOSE,
      "separator=s" => \$SEPARATOR_CHAR,
      "precision|p=i" => \$PRECISION,
      "tabfile|t=s" => \$TABFILE,
      "compare|c" => \$COMPARE,
      "union|u=s" => \$UNION,
      "help|h" => \$HELP
);

usage() unless $usagestatus;

if ($HELP) {
      usage();
    print <<EOT;
  --datadir : Specifies source directory for input files.  Default:
$DEFAULT_DATA_DIR
  --studentsfile : Specifies students file.  Default:
$DEFAULT_FILE_STUDENTS
  --workfile: Specifies work file.  Default: $DEFAULT_FILE_WORK
  --workinstancesfile: Specfies workinstances file.  Default:
$DEFAULT_FILE_WORKINSTANCES
  --themeinstancesfile: Specfies themeinstances file.  Default:
$DEFAULT_FILE_THEMEINSTANCES
  --verbose | -v: Verbose mode.  Shows extra processing info.  Default:
$DEFAULT_VERBOSE
  --separator: Separator character used internally.  Default:
$DEFAULT_SEPARATOR_CHAR
  --precision | -p: Number of decimal places to show in output.
Default: $DEFAULT_PRECISION
  --tabfile | -t: Output file for tab-separated text out.  No default.
  --help | -h: Shows this message.
EOT
}
```

```
#print "ARGV: " . join(" ",@ARGV);
#exit();
print "Version: $VERSION\n";

if ($UNION) {
      @union_workids = split(/\s+/, $UNION);
}

# Make sure the arguments supplied are all numeric.
foreach $arg (@ARGV) {
      if ($arg !~ m#\d+#) {
            print "Arguments must be numeric.\n";
        &usage();
        die(1);
      } else {
            push @itemids, $arg;
      }
}

if ($VERBOSE) {
      print <<EOT;
-----
Configuration:
      DATA_DIR = $DATA_DIR
      STUDENTSFILE = $FILE_STUDENTS
      WORKFILE = $FILE_WORK
      WORKINSTANCESFILE = $FILE_WORKINSTANCES
      THEMEINSTANCESFILES = $FILE_THEMEINSTANCES
      VERBOSE = $VERBOSE
      SEPARATOR = $SEPARATOR_CHAR
      PRECISION = $PRECISION
      TABFILE = $TABFILE
-----
EOT

}

print "Processing Instances (" . scalar @itemids . "): " . join("
",@itemids) . "\n" if $VERBOSE;
print "-----\n" if $VERBOSE;


# Link each data file with an array using Tie::File (efficient).
tie @students, 'Tie::File', $DATA_DIR . "/" . $FILE_STUDENTS, mode =>
O_RDONLY or die $!;
tie @work , 'Tie::File', $DATA_DIR . "/" . $FILE_WORK, mode => O_RDONLY
or die $!;
tie @workinstances, 'Tie::File', $DATA_DIR . "/" . $FILE_WORKINSTANCES,
mode => O_RDONLY or die $!;
tie @themeinstances, 'Tie::File', $DATA_DIR . "/" .
$FILE_THEMEINSTANCES, mode => O_RDONLY or die $!;

die "Theme instance file '$FILE_THEMEINSTANCES' only contained a single
record.  Parsing problem?  Exiting."
      unless ( scalar @themeinstances > 1 );

$tabfile_rows = "";
```

```
# Calculate our union set from the supplied workinstances.
if ($UNION) {
      $unionset = Set::Scalar->new;
      foreach $workid (@union_workids) {
      my $themeset = fetchthemeset($workid,\@themeinstances);
        $unionset = $unionset->union($themeset);
    }
    print "unionset: ", $unionset->size, "\n";

    foreach $item (@itemids) {
      my $item_themeset = fetchthemeset($item,\@themeinstances);
        my $union_themeset = $item_themeset->union($unionset);
        my $shared_themeset = $item_themeset->intersection($unionset);
        my $item_themeset_size = $item_themeset->size;
        my $union_themeset_size = $union_themeset->size;
        my $shared_themeset_size = $shared_themeset->size;
        my $similarity = $shared_themeset_size / $union_themeset_size;
      $item_allthemes = Set::Scalar->new;
      foreach $element ($item_themeset->elements) {
            my($lht,$rel,$rht) = split /$SEPARATOR_CHAR/, $element;
            $item_allthemes->insert($lht);
            $item_allthemes->insert($rht);
      }
      $item_allthemes_size = $item_allthemes->size;
        my $global_themeset = Set::Scalar->new;
      foreach $element ($union_themeset->elements) {
            my($lht,$rel,$rht) = split /$SEPARATOR_CHAR/, $element;
            $global_themeset->insert($lht);
            $global_themeset->insert($rht);
      }
      $global_themeset_size = $global_themeset->size;
      print "item($item): $item_themeset_size - ";
        print "union: $union_themeset_size - ";
      print "shared: $shared_themeset_size - ";
      print "global: $global_themeset_size ";
      print "($item:$item_allthemes_size) ";
      printf "similarity: %.${PRECISION}f\n", $similarity;

      if ($TABFILE) {
                $tabfile_rows .= "$item\t$item_themeset_size";
           $tabfile_rows .=
"\t$union_themeset_size\t$shared_themeset_size";
            $tabfile_rows .=
"\t$global_themeset_size\t$item_allthemes_size\t";
            $tabfile_rows .= sprintf("%.${PRECISION}f\n", $similarity);
        }
    }
    if ($TABFILE) {
      open (TAB, ">$TABFILE") or die "Can't open $TABFILE for writing:
$!";
      print TAB "workinstanceid1\tthemesetsize1";
      print TAB
"\tunionthemesetsize\tsharedthemesetsize\tglobalthemesetsize";
      print TAB "\titem1allthemesize\tsimilarity\n";
      print TAB "$tabfile_rows\n";
      close TAB;
      print "Saved output in $TABFILE.\n";
```

```
}

    exit;
}
# http://search.cpan.org/~jhi/Set-Scalar-1.20/lib/Set/Scalar.pm
$history = Set::Scalar->new;

# Loop through the supplied itemids twice, skipping pairs we have
already
# compared previously.
foreach $item1 (@itemids) {
      foreach $item2 (@itemids) {
            # Avoid narcissism.
            next if ($item1 == $item2);
            # Skip previous comparisons (bidirectional).
            next if ($history->has($item1 . $SEPARATOR_CHAR . $item2));
            next if ($history->has($item2 . $SEPARATOR_CHAR . $item1));
            # Fetch our themesets for the items we're comparing.
            $item1_themeset = fetchthemeset($item1,\@themeinstances);
            $item2_themeset = fetchthemeset($item2,\@themeinstances);
            # Determine the union of the two sets.
            $union_themeset = $item1_themeset->union($item2_themeset);
            # Determine the intersection of the two sets.
            $shared_themeset = $item1_themeset-
>intersection($item2_themeset);
            # Count the size of the various sets.
            $item1_themeset_size = $item1_themeset->size;
            $item2_themeset_size = $item2_themeset->size;
            $union_themeset_size = $union_themeset->size;
            $shared_themeset_size = $shared_themeset->size;

            # Explode the theme triplets from the union set into a set
of
            # unique themes.
            $global_themeset = Set::Scalar->new;
            $item1_allthemes = Set::Scalar->new;
            $item2_allthemes = Set::Scalar->new;

            foreach $element ($union_themeset->elements) {
                  my($lht,$rel,$rht) = split /$SEPARATOR_CHAR/,
$element;
                  $global_themeset->insert($lht);
                  $global_themeset->insert($rht);
            }
            $global_themeset_size = $global_themeset->size;
            foreach $element ($item1_themeset->elements) {
                  my($lht,$rel,$rht) = split /$SEPARATOR_CHAR/,
$element;
                  $item1_allthemes->insert($lht);
                  $item1_allthemes->insert($rht);
            }
            $item1_allthemes_size = $item1_allthemes->size;
            foreach $element ($item2_themeset->elements) {
                  my($lht,$rel,$rht) = split /$SEPARATOR_CHAR/,
$element;
                  $item2_allthemes->insert($lht);
                  $item2_allthemes->insert($rht);
            }
```

```
            $item2_allthemes_size = $item2_allthemes->size;

            $similarity = $shared_themeset_size / $union_themeset_size;

            print "item($item1): $item1_themeset_size - ";
            print "item($item2): $item2_themeset_size - ";
            print "union: $union_themeset_size - ";
            print "shared: $shared_themeset_size - ";
            print "global: $global_themeset_size ";
            print "($item1:$item1_allthemes_size) ";
            print "($item2:$item2_allthemes_size) - ";
            printf "similarity: %.${PRECISION}f\n", $similarity;

        if ($TABFILE) {
                $tabfile_rows .=
"$item1\t$item1_themeset_size\t$item2\t$item2_themeset_size";
          $tabfile_rows .=
"\t$union_themeset_size\t$shared_themeset_size";
            $tabfile_rows .=
"\t$item1_allthemes_size\t$item2_allthemes_size\t$global_themeset_size\
t";
            $tabfile_rows .= sprintf("%.${PRECISION}f\n", $similarity);
        }
            #print "global themeset: ", $global_themeset, "\n";

            # Add the comparison to our history.
            $history->insert($item1 . $SEPARATOR_CHAR . $item2);
      }
}

if ($TABFILE) {
      open (TAB, ">$TABFILE") or die "Can't open $TABFILE for writing:
$!";
    print TAB
"workinstanceid1\tthemesetsize1\tworkinstanceid2\tthemesetsize2";
    print TAB "\tunionthemesetsize\tsharedthemesetsize";
    print TAB
"\titem1allthemesize\titem2allthemesize\tglobalthemesetsize\tsimilarity
\n";
      print TAB "$tabfile_rows\n";
    close TAB;
    print "Saved output in $TABFILE.\n";
}

exit(0);

# Return a set containing the theme/relation/theme triplets for the
supplied
# work instance ID.
sub fetchthemeset {
      ($workinstanceid, $itemarrayref) = @_;
      $set = Set::Scalar->new;

      # Iterate over each line of the referenced array (which is really
our
      # tied database file.
      foreach $line (@$itemarrayref) {
            # Split each line on the delimiter (tab).
```

```
            my($rowid,$winstcid,$lht,$rht,$rel,$workid,$studentid) =
split /\t/, $line;
            # Only select those lines for our selected work instance
ID.
            next unless ($winstcid == $workinstanceid);
            # Insert this theme triplet into our set.
            $set->insert($lht . $SEPARATOR_CHAR . $rel .
$SEPARATOR_CHAR . $rht);
      }
      return $set;
}
# END PROGRAM
```

## APPENDIX D: IRB APPROVAL

THE UNIVERSITY OF MICHIGAN

OFFICE OF THE VICE PRESIDENT FOR RESEARCH

BEHAVORIAL SCIENCES INSTITUTIONAL REVIEW BOARD
HEALTH SCIENCES INSTITUTIONAL REVIEW BOARD
1042 FLEMING BUILDING, 503 THOMPSON STREET
ANN ARBOR, MICHIGAN 48109-1340
PHONE: 734 936-0933 FAX: 734 647-9084
E-MAIL: irbhsbs@umich.edu WEBSITE: www.irb.research.umich.edu

Mr. Alan Kiste
LS&A Chemistry Department
Chem 2408
Department of Chemistry
1055

Dear Mr. Kiste:

**The Behavioral Sciences Institutional Review Board (IRB) has reviewed and approved your research proposal involving human subjects.** The IRB determined that the research and its procedures are compliant with appropriate guidelines, state and federal regulations, and the University of Michigan's Federal Wide Assurance (FWA00004969 Expiration 6/12/06) on file with the Department of Health and Human Services (HHS).

**Please remember that approval must be obtained for changes in procedures or consent document(s) related to your research proposal.** If changes are contemplated, they must be approved prior to initiation of the modified procedures.

**The approval period for this project is for a period of one year from the approval date listed below, or a shorter period, if specified.** *Please note your expiration date.* Approximately three months prior to the expiration date, you will be notified so that your renewal application can be prepared, submitted, and reviewed in a timely manner without interruption in the approval status of this project. You must allow up to six weeks for the review process. **If you allow your approval to lapse, no work may be conducted on this project until appropriate approval has been obtained.**

**You are also required to inform the IRB of all unanticipated or adverse events** (i.e., physical, social, or emotional injury) as soon as possible after the event. The forms necessary for modifications and adverse event reporting can be obtained on the IRB website at http://www.irb.research.umich.edu.

Sincerely,

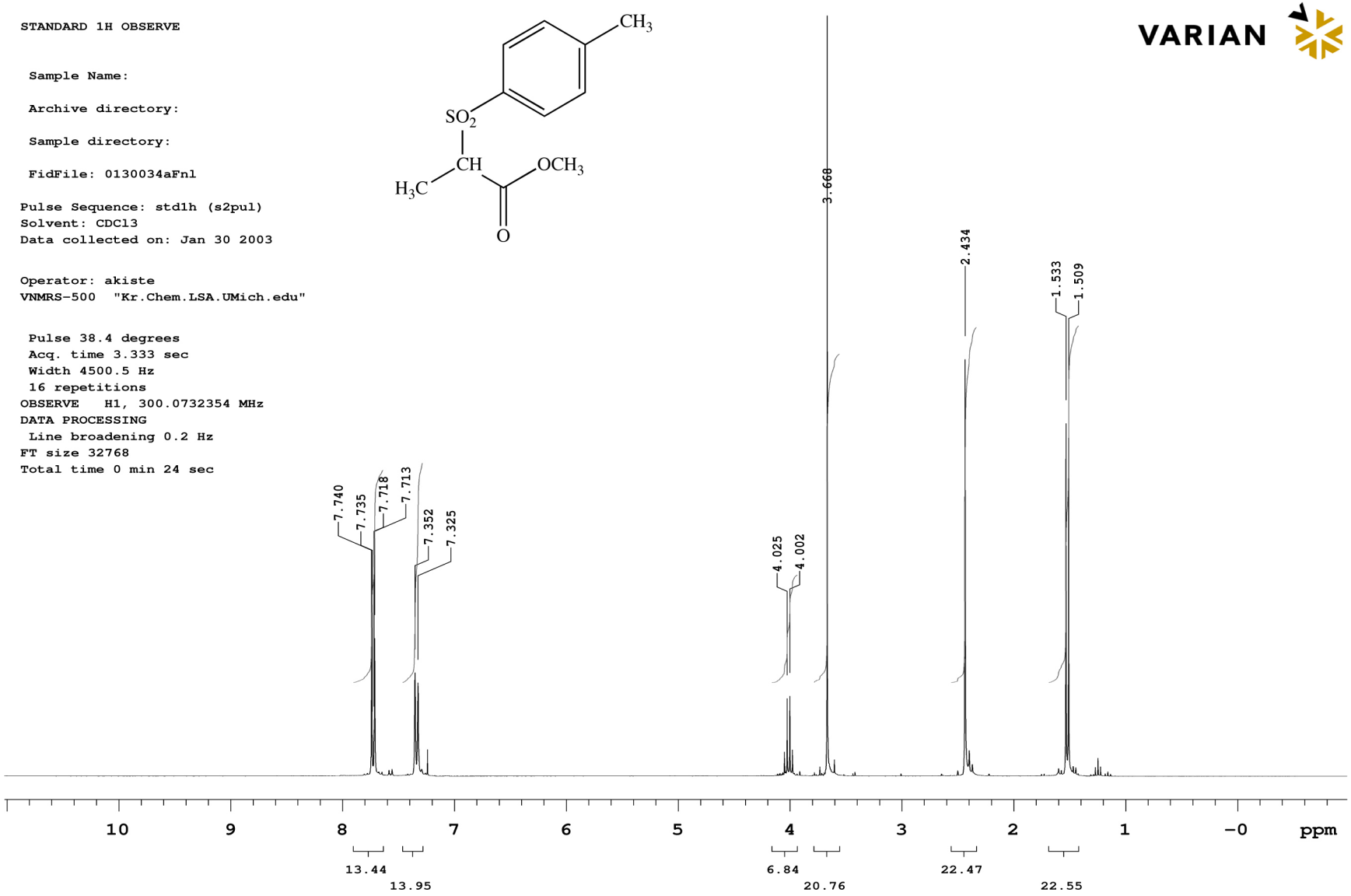
John O'Shea, Ph.D.
Co-chair, Behavioral Sciences Institutional Review Board

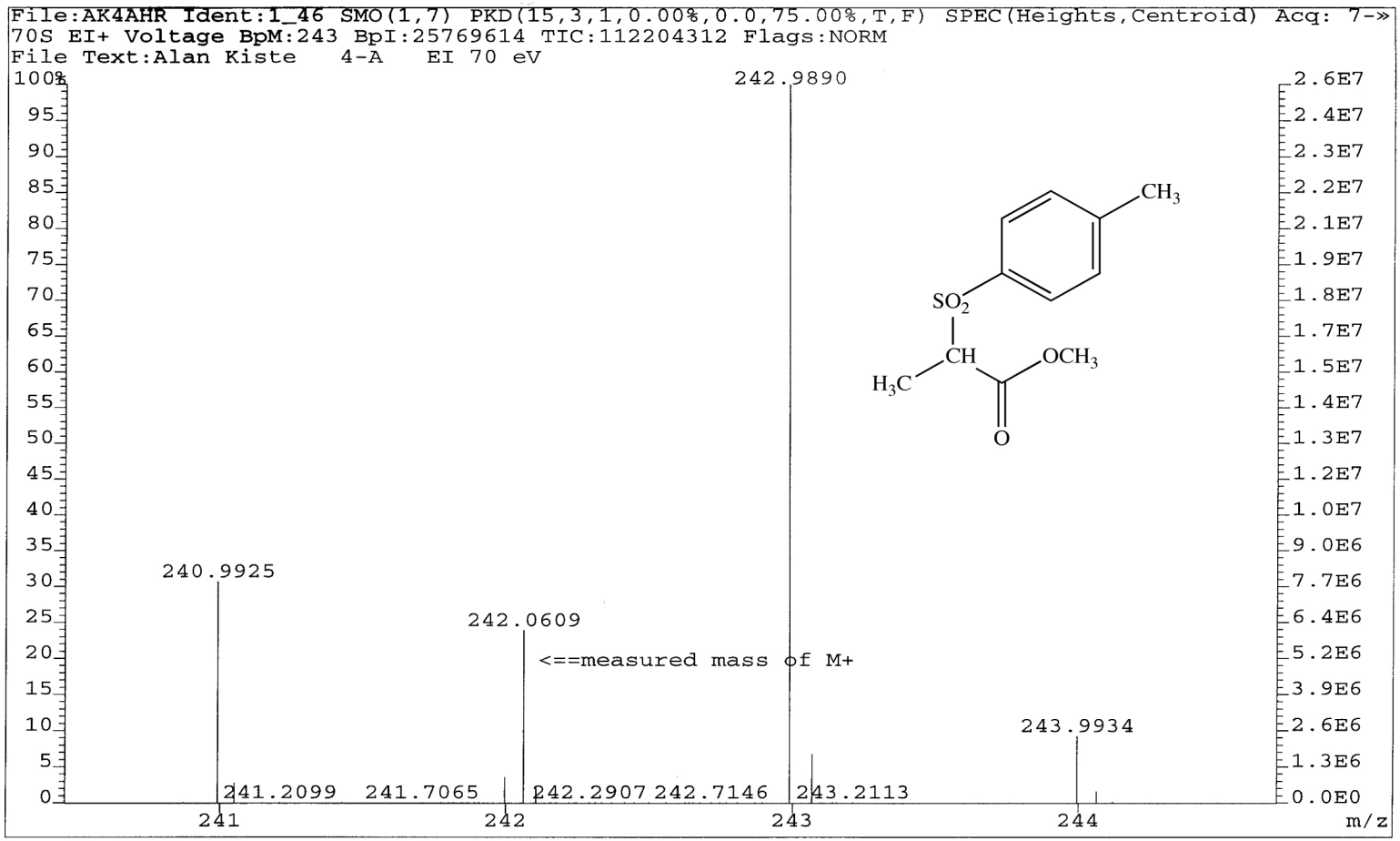
cc: DRDA

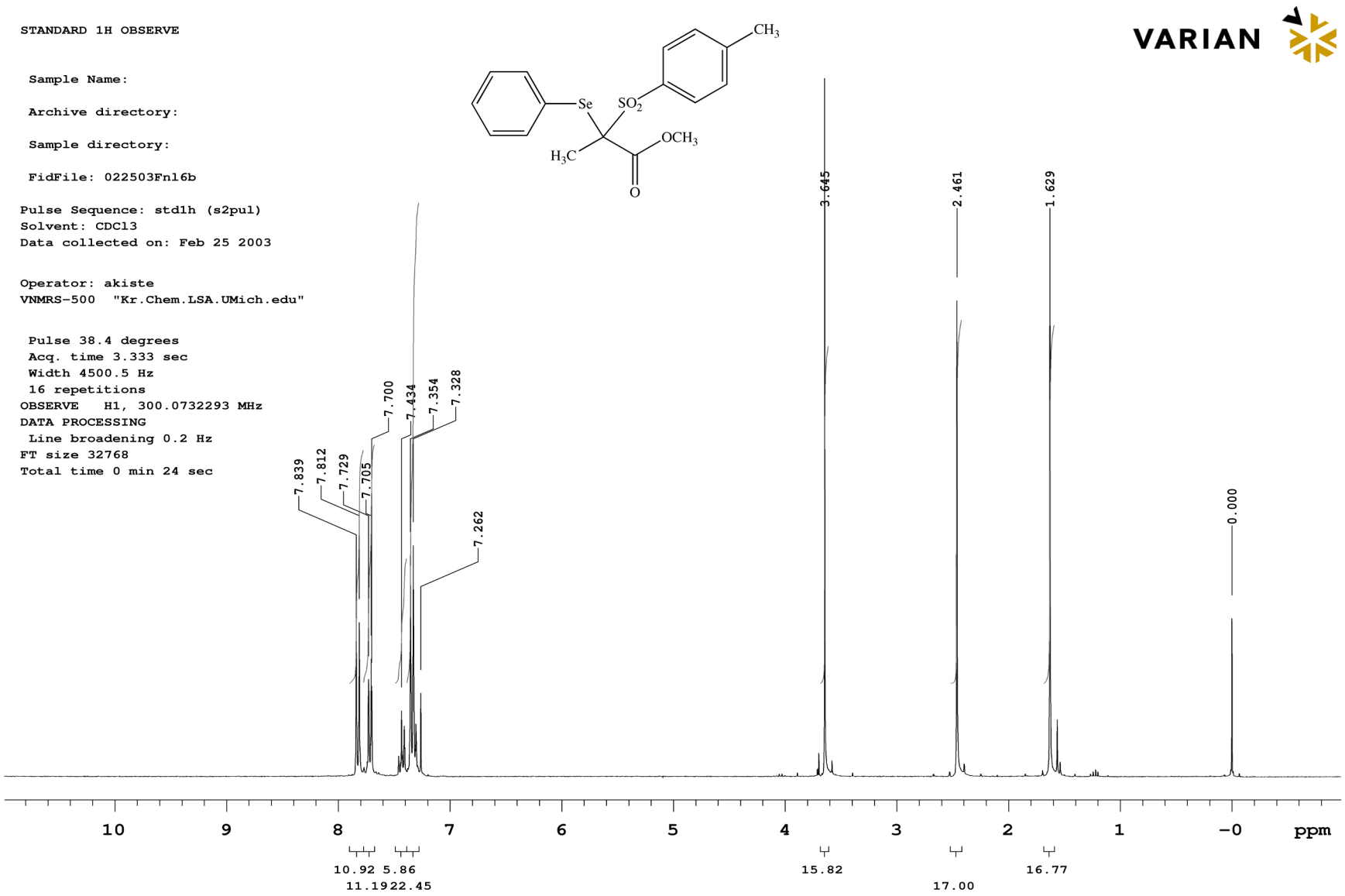
PROJECT TITLE: Examining chemistry students' representational abilities
PROJECT APPROVAL DATE: 12/16/2004 TO EXPIRATION DATE: EXEMPT
SOURCE OF FUNDS: N/A, N/A
IRB FILE NUMBER: B04-00006530-I

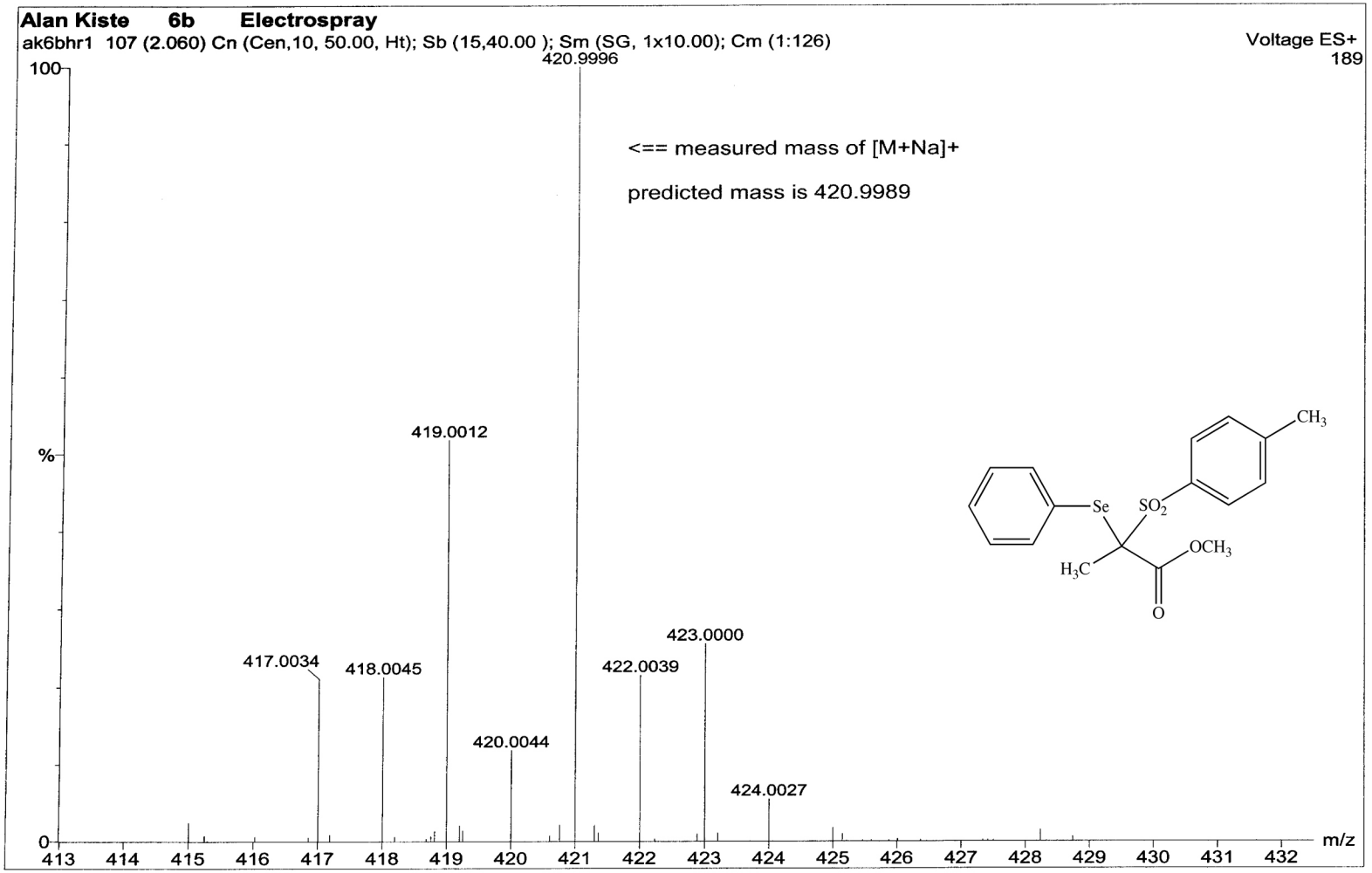
To obtain related documents: http://www.irb.research.umich.edu

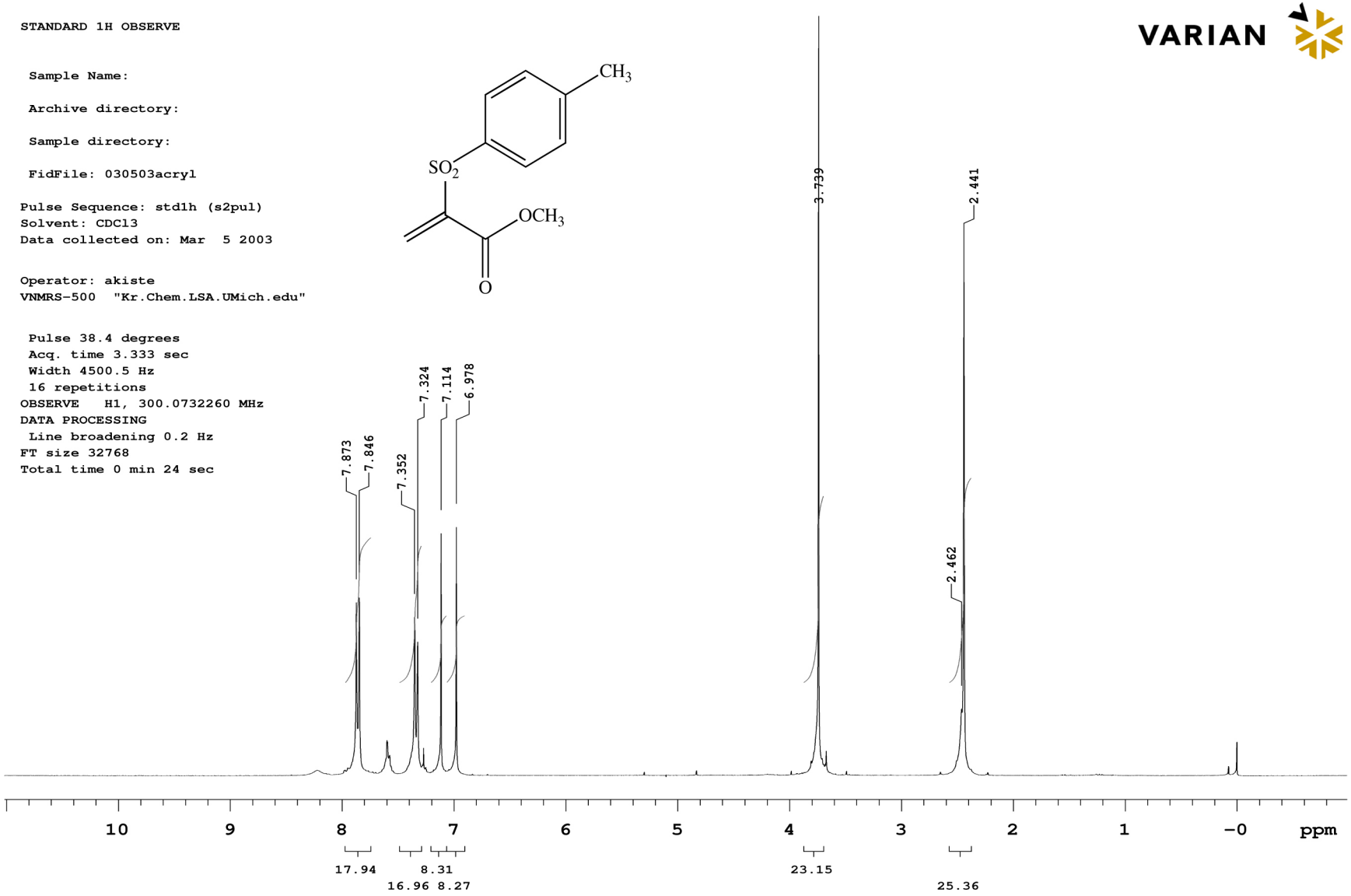
# APPENDIX E: SPECTRA

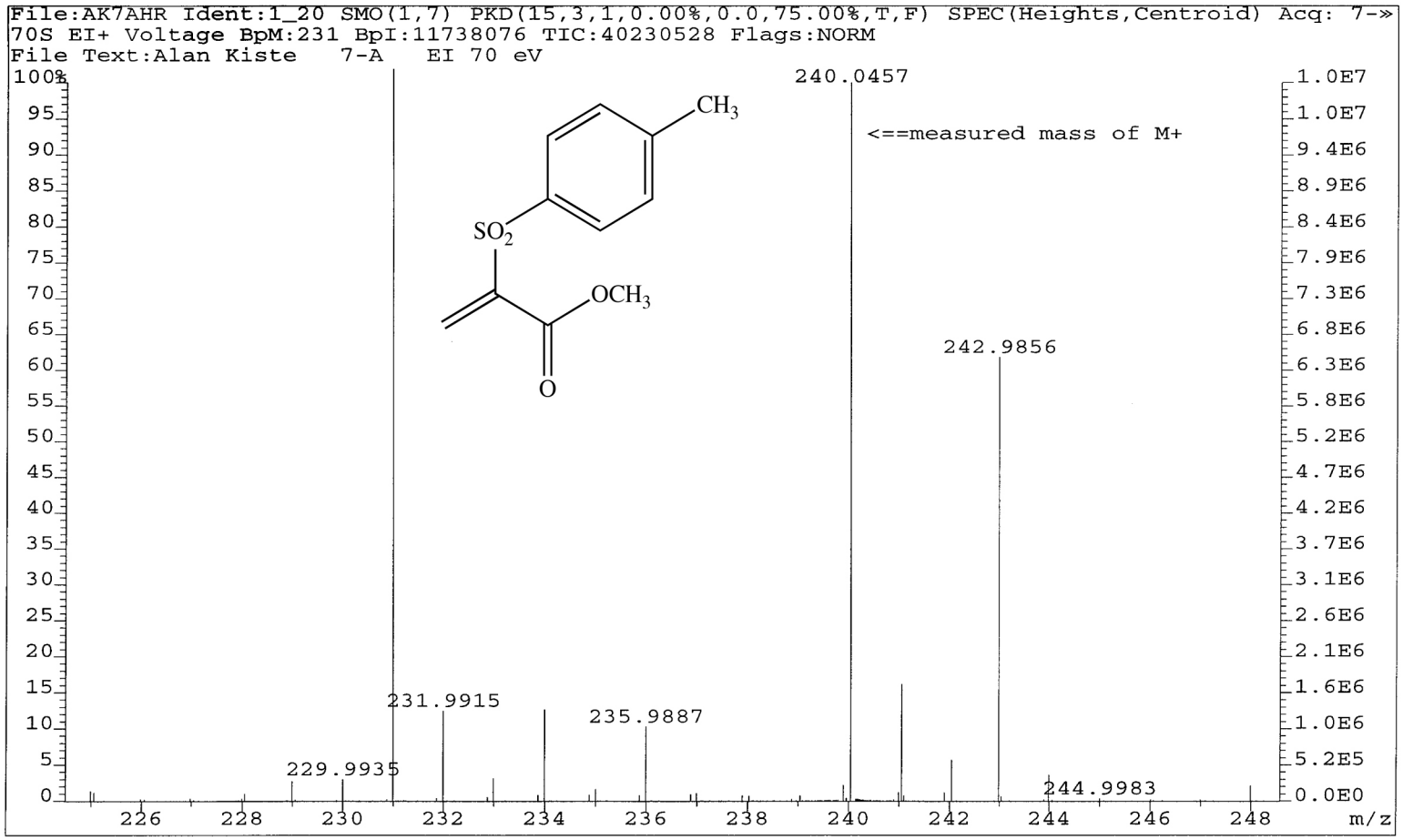

STANDARD 1H OBSERVE
Sample Name:
Archive directory:
Sample directory:
FidFile: 0130034aFnl
Pulse Sequence: std1h (s2pul)
Solvent: CDCl3
Data collected on: Jan 30 2003
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Pulse 38.4 degrees
Acq. time 3.333 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0732354 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min 24 sec
VARIAN
7.740
7.735
7.718
7.713
7.352
7.325
4.025
4.002
3.668
2.434
1.533
1.509
10
9
8
7
6
5
4
3
2
1
-0
ppm
13.44
13.95
6.84
20.76
22.47
22.55

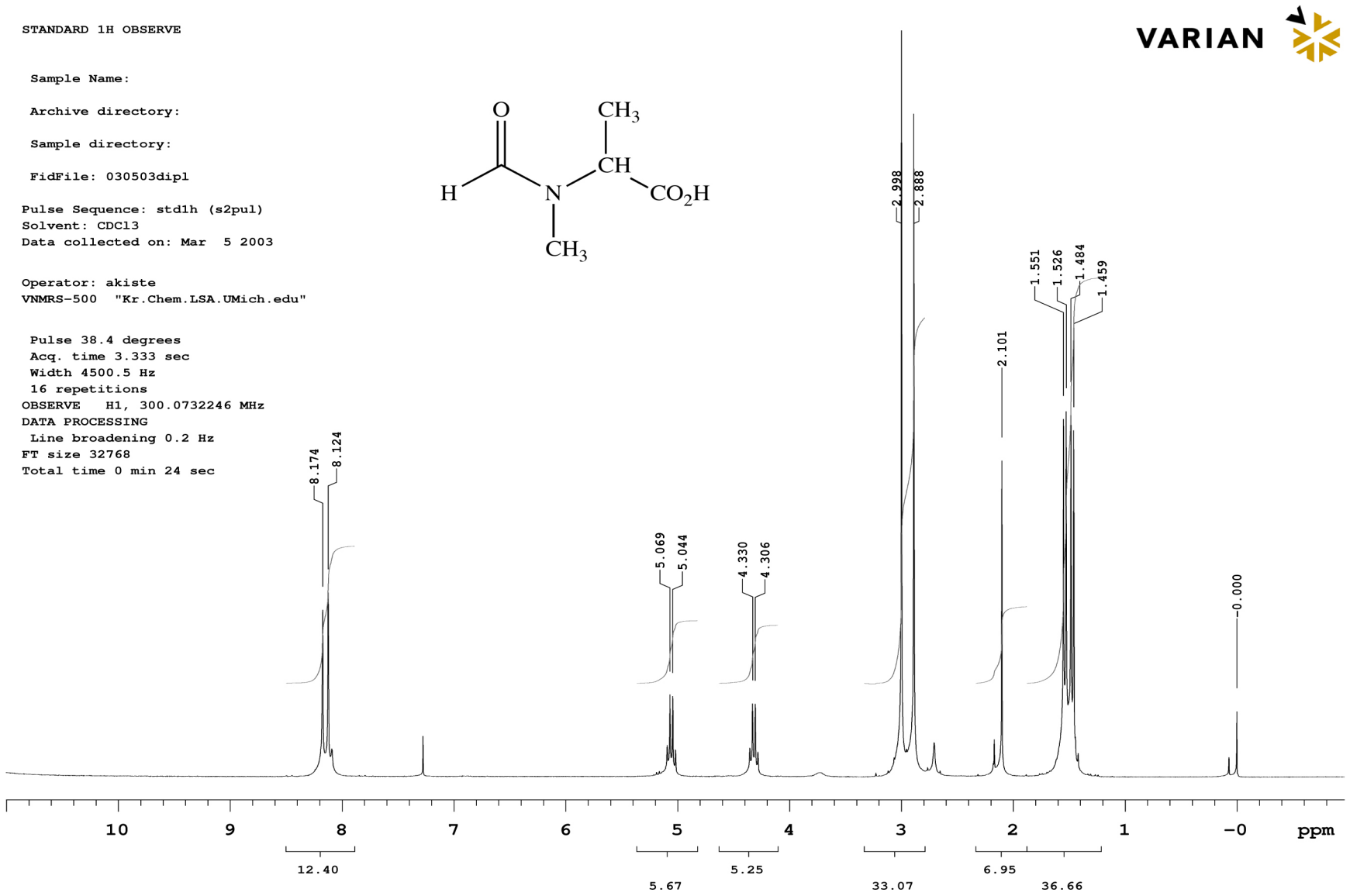

File:AK4AHR Ident:1_46 SMO(1,7) PKD(15,3,1,0.00%,0.0,75.00%,T,F) SPEC(Heights,Centroid) Acq: 7-»
70S EI+ Voltage BpM:243 BpI:25769614 TIC:112204312 Flags:NORM
File Text:Alan Kiste 4-A EI 70 eV
242.9890
240.9925
242.0609
<==measured mass of M+
243.9934
241.2099
241.7065
242.2907
242.7146
243.2113
CH3
SO2
CH
OCH3
H3C
O
m/z

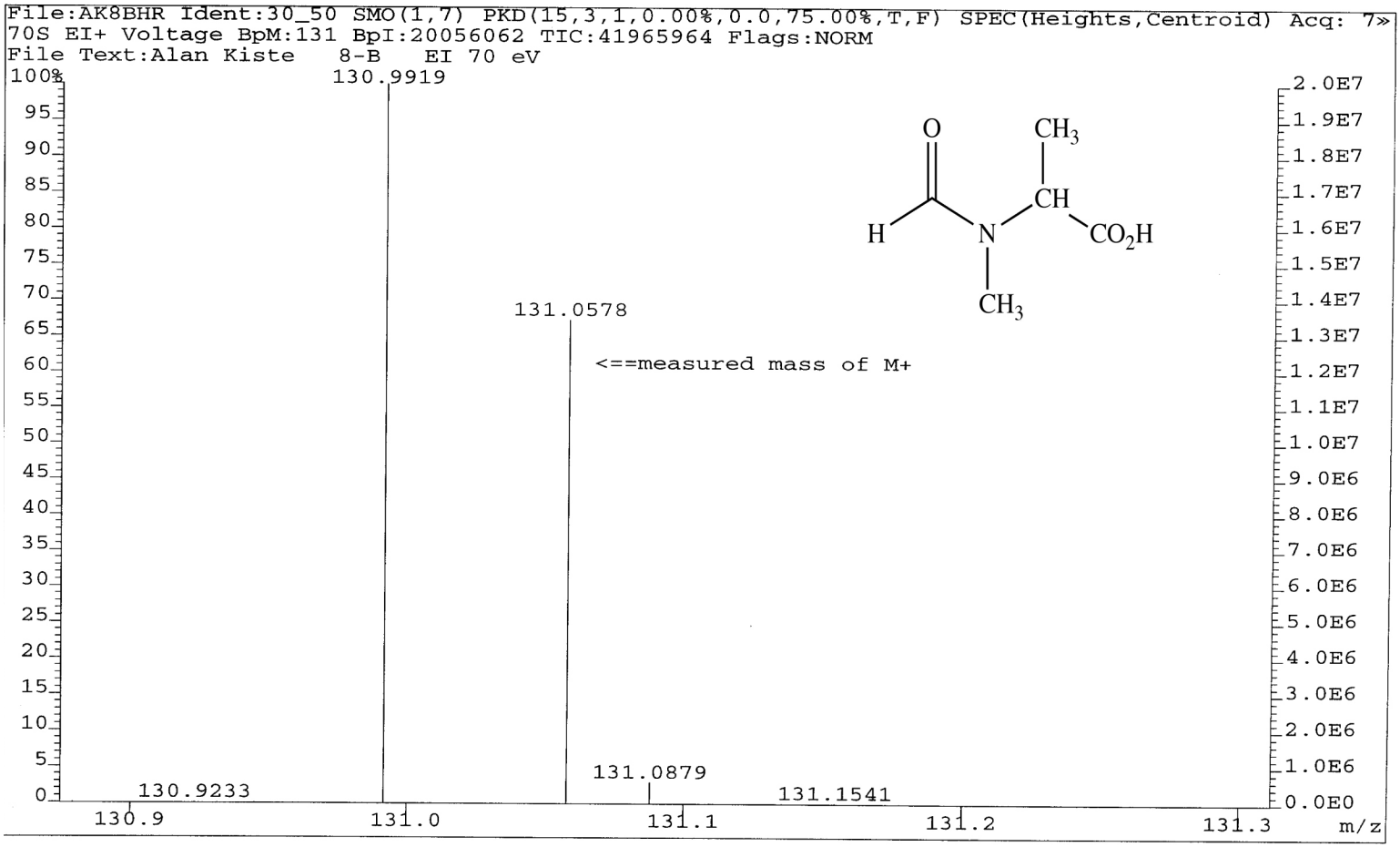

STANDARD 1H OBSERVE
Sample Name:
Archive directory:
Sample directory:
FidFile: 022503Fnl6b
Pulse Sequence: std1h (s2pul)
Solvent: CDCl3
Data collected on: Feb 25 2003
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Pulse 38.4 degrees
Acq. time 3.333 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0732293 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min 24 sec
VARIAN
Se
SO2
CH3
H3C
OCH3
O
7.839
7.812
7.729
7.705
7.700
7.434
7.354
7.328
7.262
3.645
2.461
1.629
0.000
10
9
8
7
6
5
4
3
2
1
-0
ppm
10.92
5.86
11.19
22.45
15.82
17.00
16.77

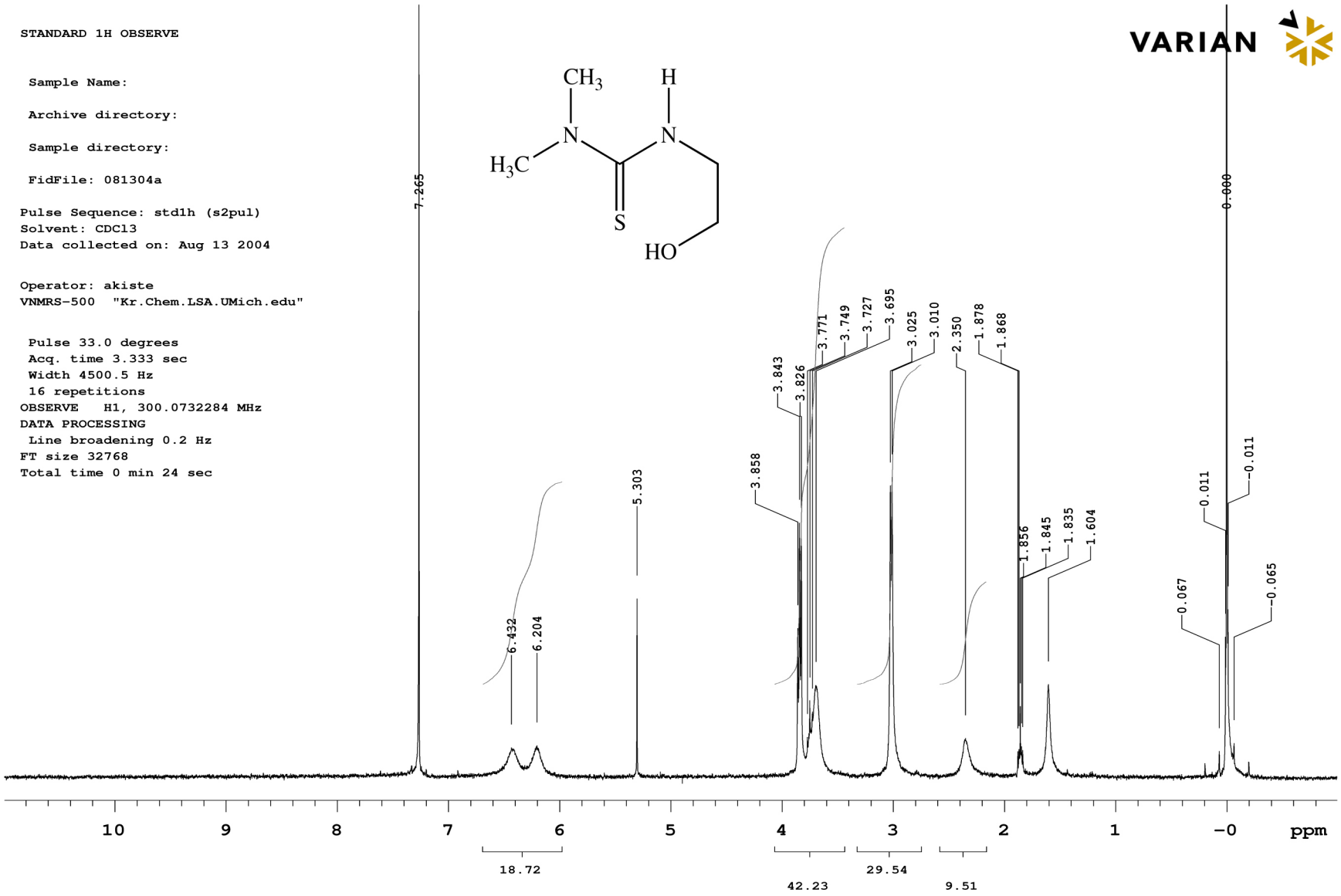

Alan Kiste 6b Electrospray
ak6bhr1 107 (2.060) Cn (Cen,10, 50.00, Ht); Sb (15,40.00 ); Sm (SG, 1x10.00); Cm (1:126)
Voltage ES+
189
100
%
0
420.9996
<== measured mass of [M+Na]+
predicted mass is 420.9989
419.0012
417.0034
418.0045
420.0044
422.0039
423.0000
424.0027
413 414 415 416 417 418 419 420 421 422 423 424 425 426 427 428 429 430 431 432
m/z
CH3
Se
SO2
OCH3
H3C
O

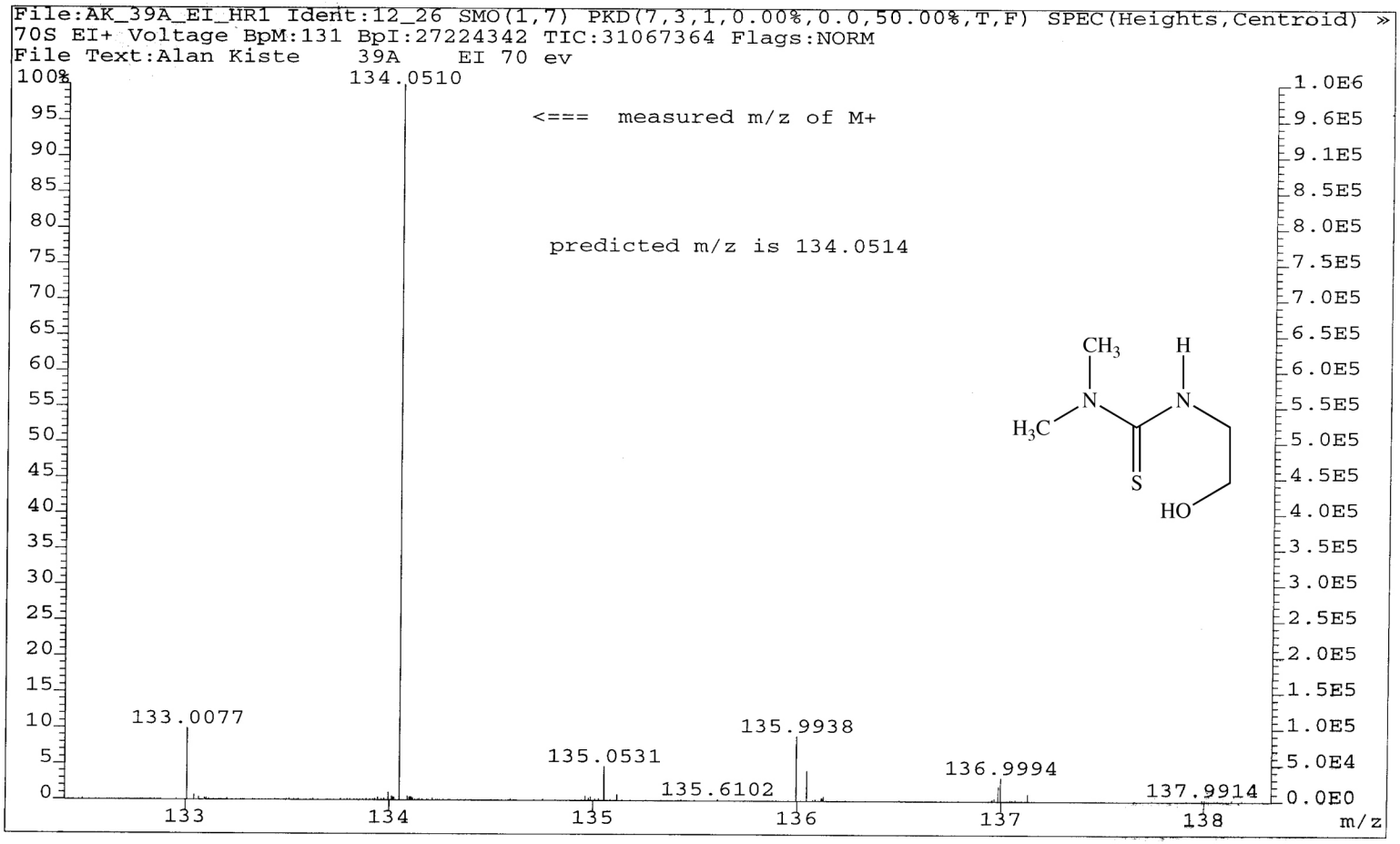

STANDARD 1H OBSERVE
Sample Name:
Archive directory:
Sample directory:
FidFile: 030503acryl
Pulse Sequence: std1h (s2pul)
Solvent: CDCl3
Data collected on: Mar 5 2003
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Pulse 38.4 degrees
Acq. time 3.333 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0732260 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min 24 sec
CH3
SO2
OCH3
O
VARIAN
7.873
7.846
7.352
7.324
7.114
6.978
3.739
2.462
2.441
10
9
8
7
6
5
4
3
2
1
-0
ppm
17.94
8.31
16.96
8.27
23.15
25.36

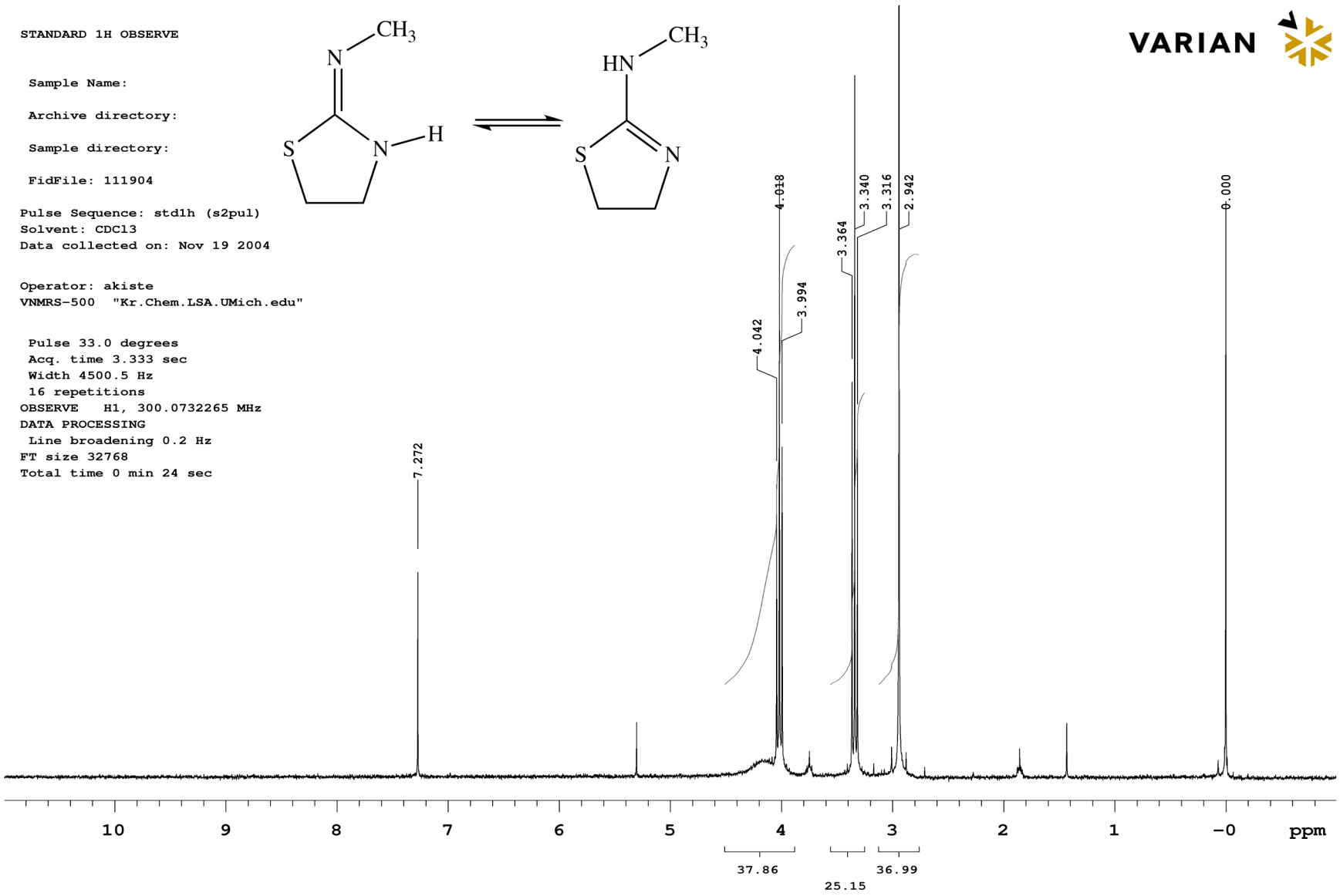

File:AK7AHR Ident:1_20 SMO(1,7) PKD(15,3,1,0.00%,0.0,75.00%,T,F) SPEC(Heights,Centroid) Acq: 7-»
70S EI+ Voltage BpM:231 BpI:11738076 TIC:40230528 Flags:NORM
File Text:Alan Kiste 7-A EI 70 eV
240.0457
<==measured mass of M+
242.9856
231.9915
235.9887
229.9935
244.9983
CH3
SO2
OCH3
O
m/z

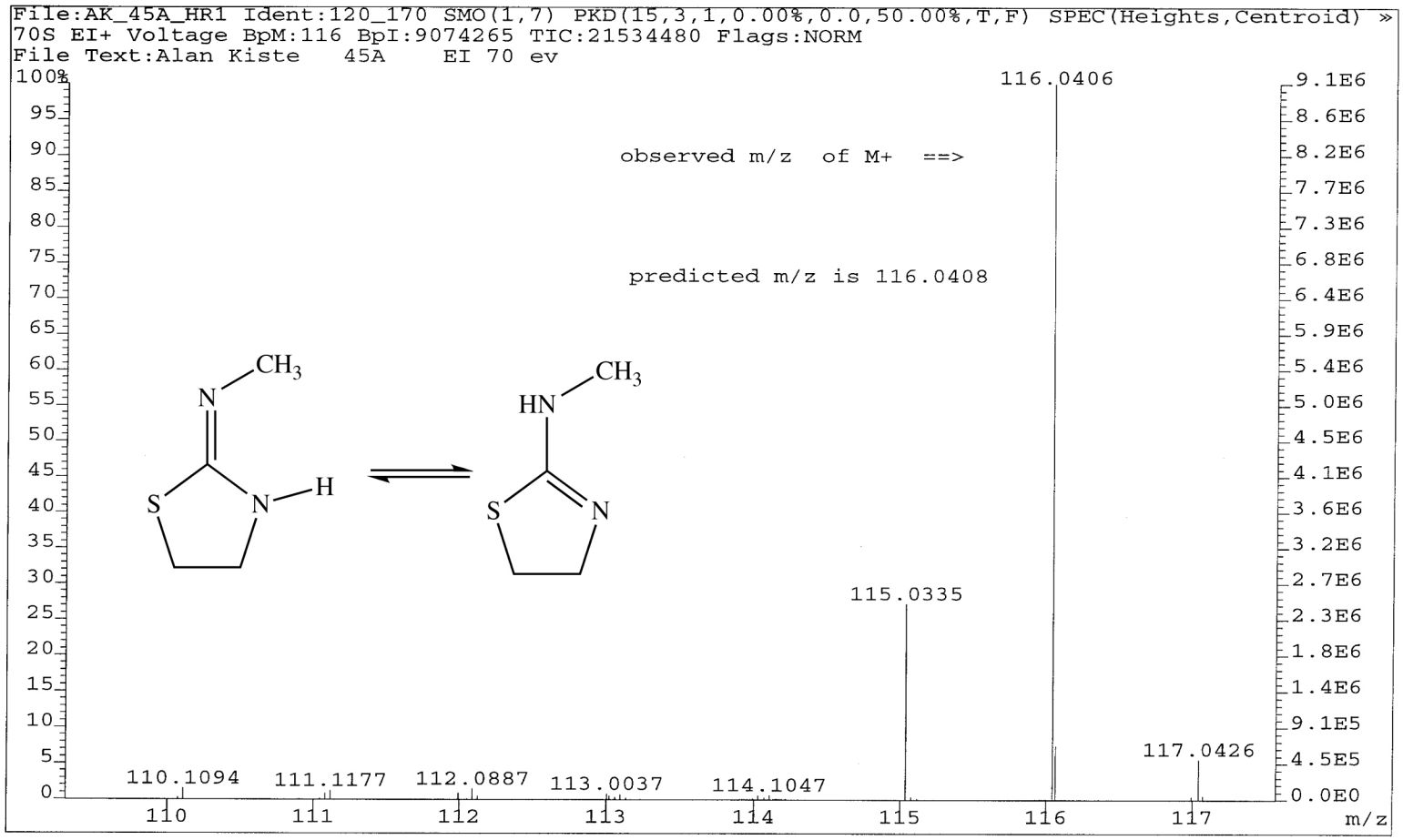

STANDARD 1H OBSERVE
Sample Name:
Archive directory:
Sample directory:
FidFile: 030503dipl
Pulse Sequence: std1h (s2pul)
Solvent: CDCl3
Data collected on: Mar 5 2003
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Pulse 38.4 degrees
Acq. time 3.333 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0732246 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min 24 sec
VARIAN
O
CH3
CH
H
N
CO2H
CH3
8.174
8.124
5.069
5.044
4.330
4.306
2.998
2.888
2.101
1.551
1.526
1.484
1.459
0.000
10
9
8
7
6
5
4
3
2
1
-0
ppm
12.40
5.67
5.25
33.07
6.95
36.66


File:AK8BHR Ident:30_50 SMO(1,7) PKD(15,3,1,0.00%,0.0,75.00%,T,F) SPEC(Heights,Centroid) Acq: 7»
70S EI+ Voltage BpM:131 BpI:20056062 TIC:41965964 Flags:NORM
File Text:Alan Kiste 8-B EI 70 eV
130.9919
131.0578
<==measured mass of M+
130.9233
131.0879
131.1541
O
CH3
CH
H
N
CO2H
CH3
100%
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
2.0E7
1.9E7
1.8E7
1.7E7
1.6E7
1.5E7
1.4E7
1.3E7
1.2E7
1.1E7
1.0E7
9.0E6
8.0E6
7.0E6
6.0E6
5.0E6
4.0E6
3.0E6
2.0E6
1.0E6
0.0E0
130.9
131.0
131.1
131.2
131.3
m/z


STANDARD 1H OBSERVE
Sample Name:
Archive directory:
Sample directory:
FidFile: 081304a
Pulse Sequence: std1h (s2pul)
Solvent: CDCl3
Data collected on: Aug 13 2004
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Pulse 33.0 degrees
Acq. time 3.333 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0732284 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min 24 sec
VARIAN
CH3
H
N
N
H3C
S
HO
7.265
0.000
6.432
6.204
5.303
3.858
3.843
3.826
3.771
3.749
3.727
3.695
3.025
3.010
2.350
1.878
1.868
1.856
1.845
1.835
1.604
0.067
0.011
0.011
0.065
10
9
8
7
6
5
4
3
2
1
−0
ppm
18.72
42.23
29.54
9.51


File:AK_39A_EI_HR1 Ident:12_26 SMO(1,7) PKD(7,3,1,0.00%,0.0,50.00%,T,F) SPEC(Heights,Centroid) »
70S EI+ Voltage BpM:131 BpI:27224342 TIC:31067364 Flags:NORM
File Text:Alan Kiste 39A EI 70 ev
134.0510
<=== measured m/z of M+
predicted m/z is 134.0514
133.0077
135.0531
135.6102
135.9938
136.9994
137.9914
m/z


STANDARD 1H OBSERVE
Sample Name:
Archive directory:
Sample directory:
FidFile: 111904
Pulse Sequence: std1h (s2pul)
Solvent: CDCl3
Data collected on: Nov 19 2004
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Pulse 33.0 degrees
Acq. time 3.333 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0732265 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min 24 sec
VARIAN
7.272
4.042
4.018
3.994
3.364
3.340
3.316
2.942
0.000
10
9
8
7
6
5
4
3
2
1
-0
ppm
37.86
25.15
36.99


File:AK_45A_HR1 Ident:120_170 SMO(1,7) PKD(15,3,1,0.00%,0.0,50.00%,T,F) SPEC(Heights,Centroid) »
70S EI+ Voltage BpM:116 BpI:9074265 TIC:21534480 Flags:NORM
File Text:Alan Kiste 45A EI 70 ev
observed m/z of M+ ==>
predicted m/z is 116.0408
116.0406
115.0335
117.0426
110.1094
111.1177
112.0887
113.0037
114.1047
m/z

STANDARD 1H OBSERVE

Sample Name:

Archive directory:

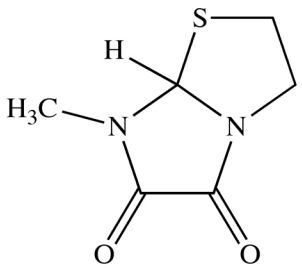
Sample directory:

FidFile: 033005a

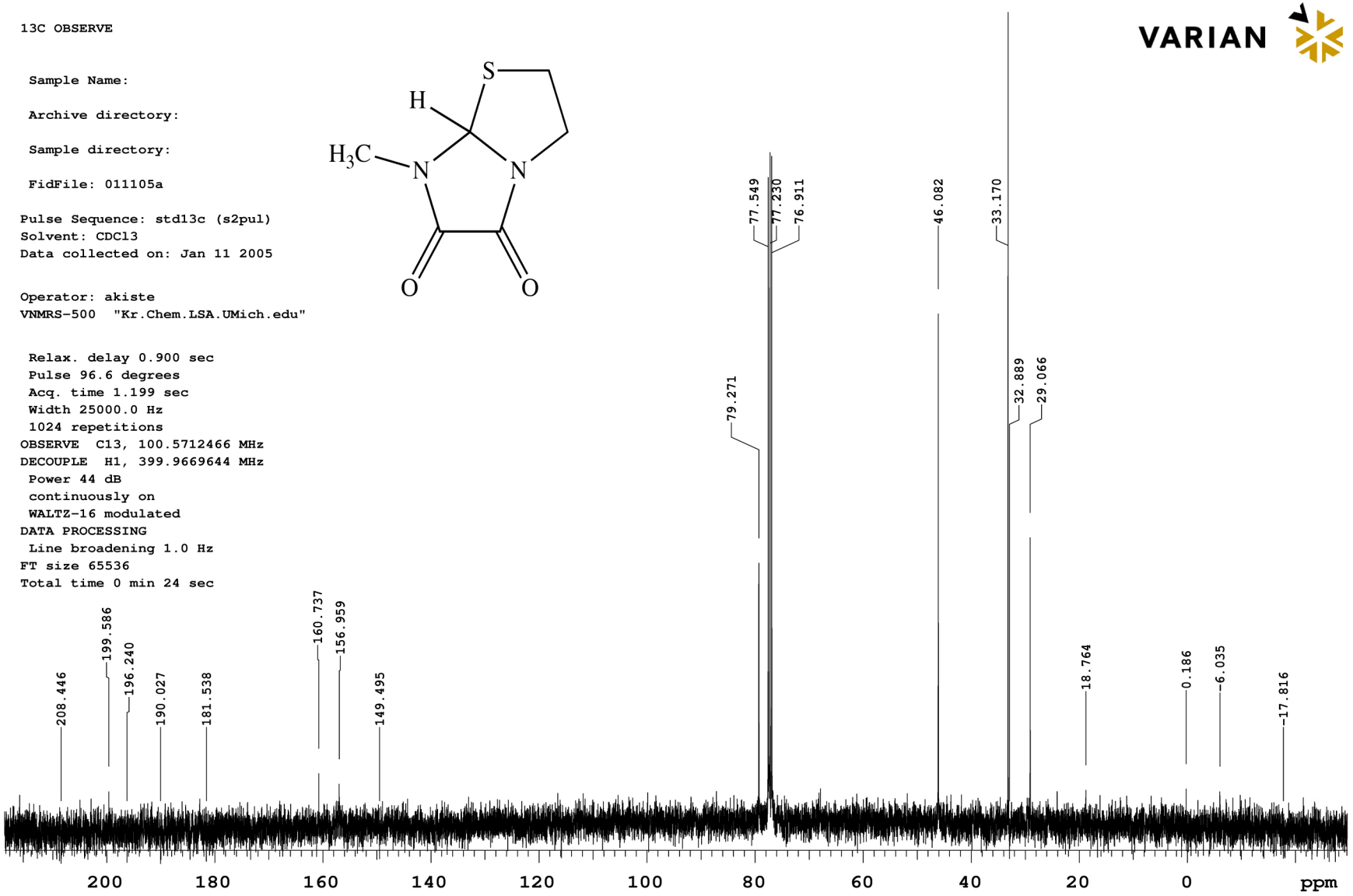
Pulse Sequence: std1h (s2pul)
Solvent: CDCl3
Data collected on: Mar 30 2005

Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"

Pulse 38.4 degrees
Acq. time 3.333 sec
Width 4500.5 Hz
16 repetitions
OBSERVE H1, 300.0732111 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min 24 sec




VARIAN


13C OBSERVE
Sample Name:
Archive directory:
Sample directory:
FidFile: 011105a
Pulse Sequence: std13c (s2pul)
Solvent: CDCl3
Data collected on: Jan 11 2005
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Relax. delay 0.900 sec
Pulse 96.6 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
1024 repetitions
OBSERVE C13, 100.5712466 MHz
DECOUPLE H1, 399.9669644 MHz
Power 44 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 0 min 24 sec
VARIAN
S
H
H3C
N
N
O
O
208.446
199.586
196.240
190.027
181.538
160.737
156.959
149.495
79.271
77.549
77.230
76.911
46.082
33.170
32.889
29.066
18.764
0.186
-6.035
-17.816
200
180
160
140
120
100
80
60
40
20
0
ppm

13C OBSERVE

Sample Name:

Archive directory:

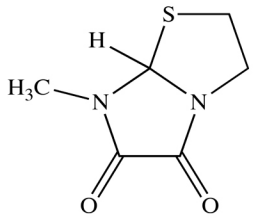
Sample directory:

FidFile: 011405a

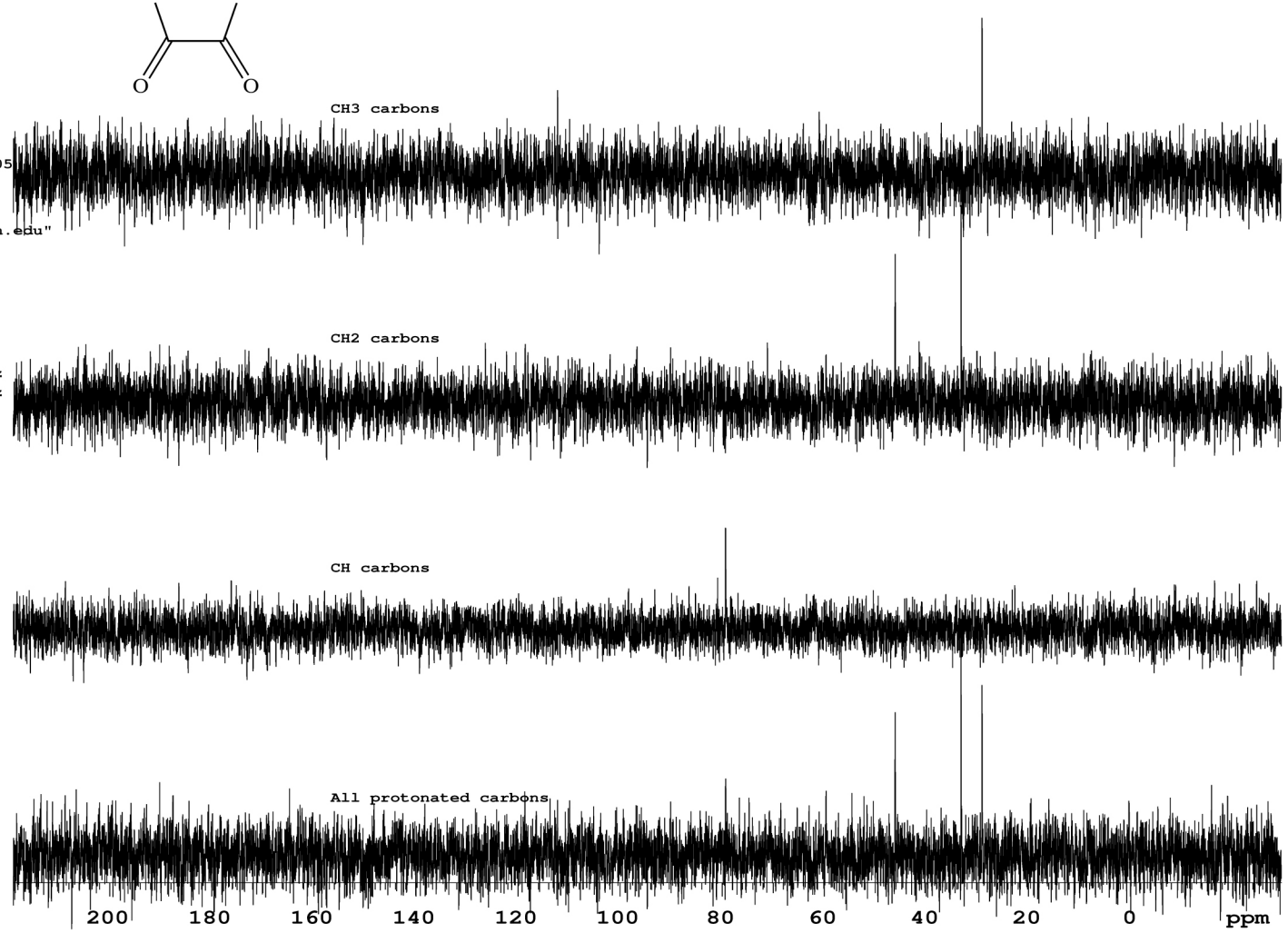
Pulse Sequence: dept
Solvent: cdcl3
Data collected on: Jan 14 2005

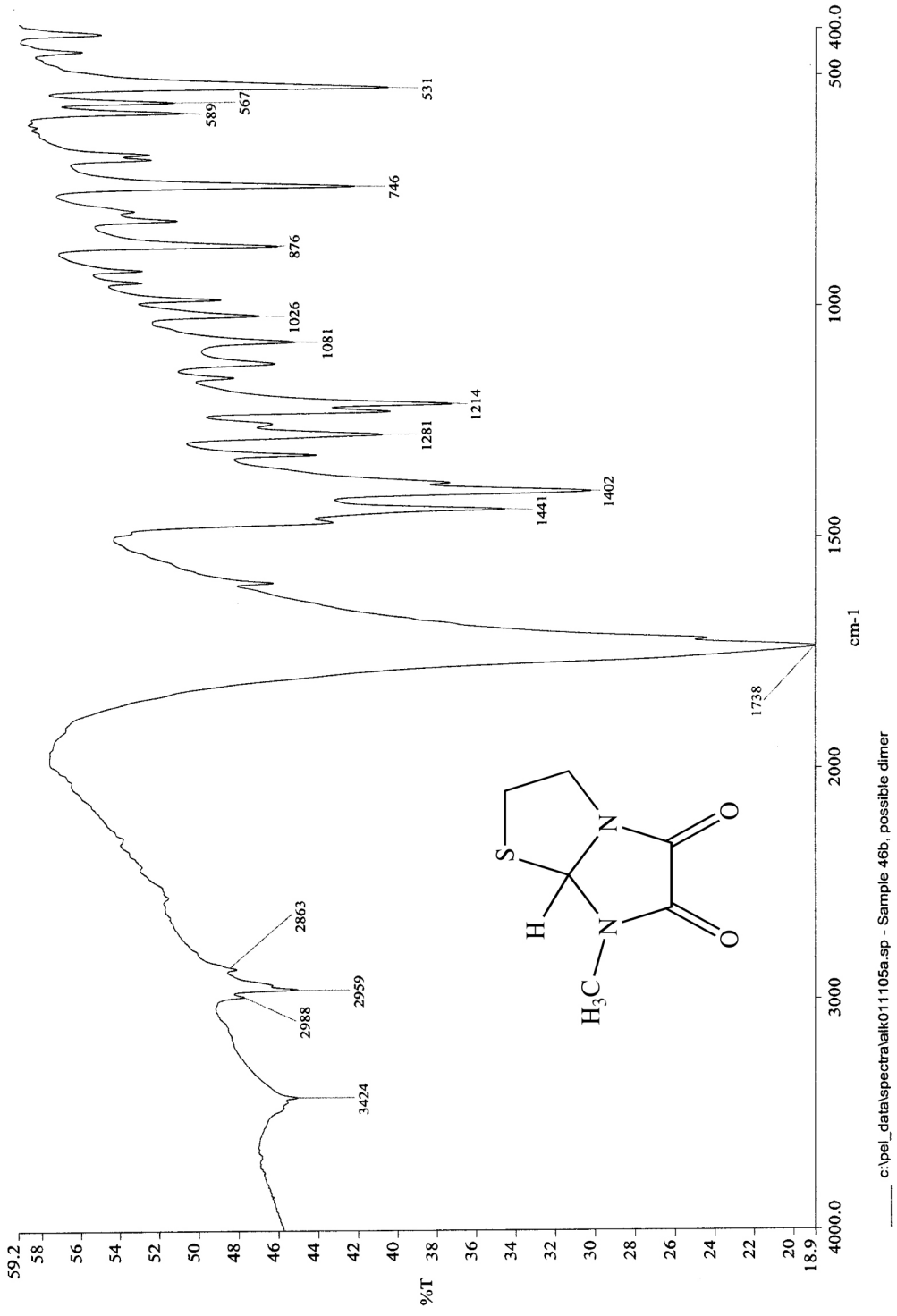
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"

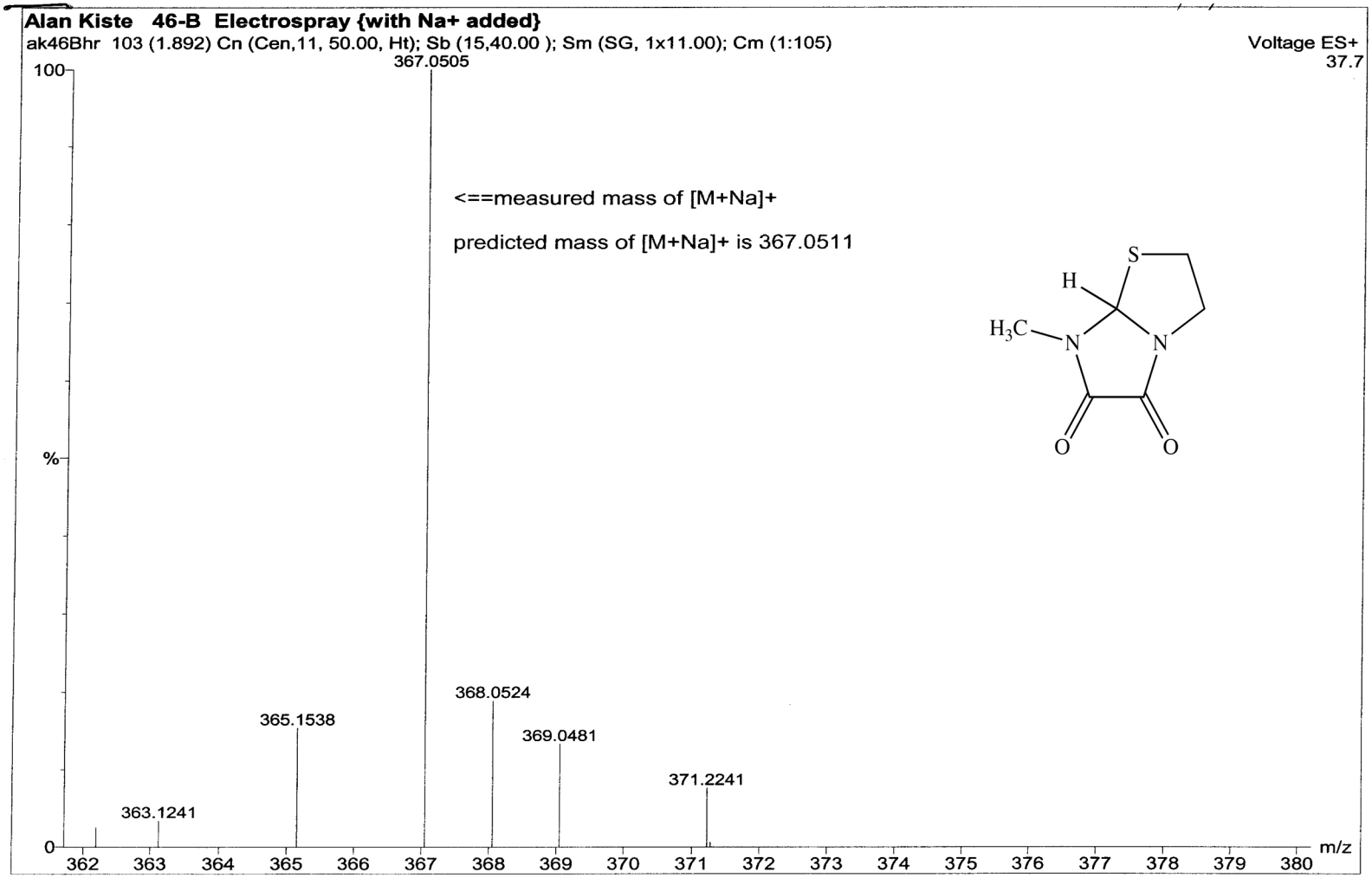
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
16 repetitions
OBSERVE C13, 100.5712463 MHz
DECOUPLE H1, 399.9669644 MHz
Power 44 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.5 Hz
FT size 131072
Total time 0 min 24 sec

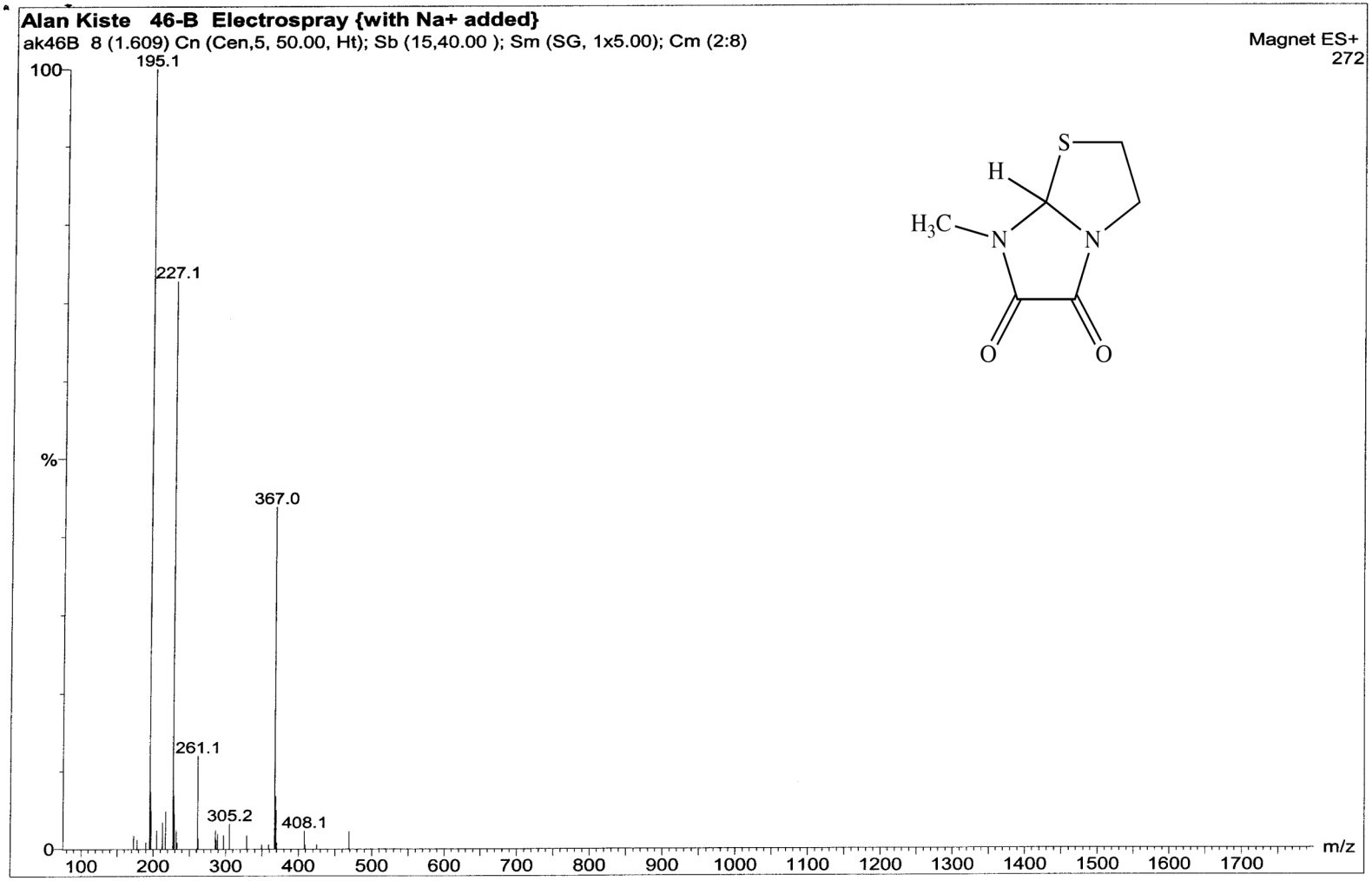


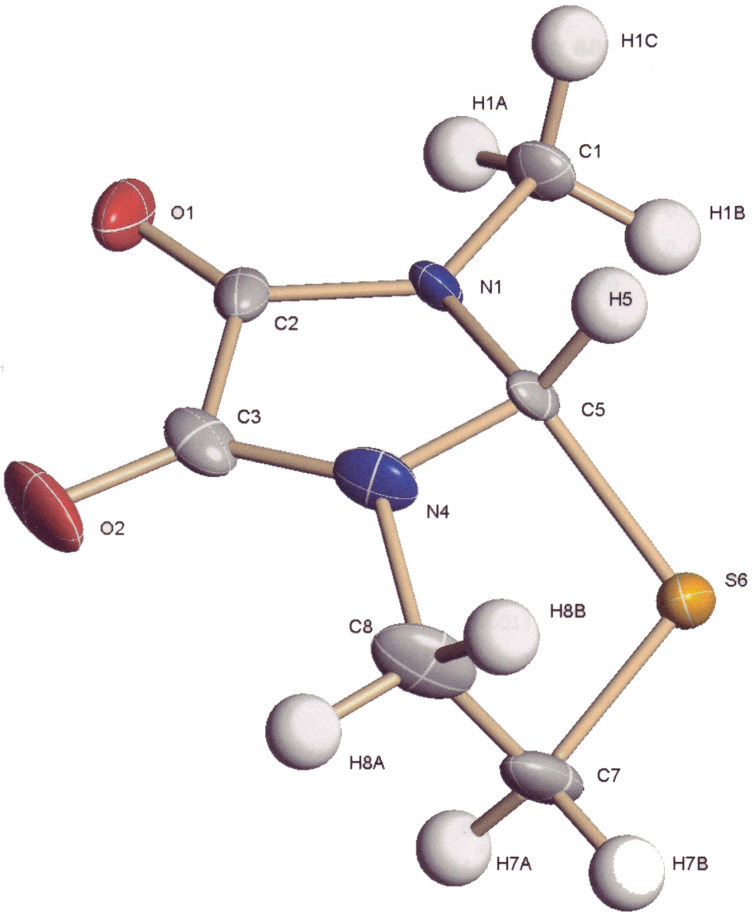

VARIAN




%T
cm-1
3424
2988
2959
2863
1738
1441
1402
1281
1214
1081
1026
876
746
589
567
531
S
N
N
O
O
H
$H_3C$
c:\pel_data\spectra\alk011105a.sp - Sample 46b, possible dimer


Alan Kiste 46-B Electrospray {with Na+ added}
ak46Bhr 103 (1.892) Cn (Cen,11, 50.00, Ht); Sb (15,40.00 ); Sm (SG, 1x11.00); Cm (1:105)
Voltage ES+
37.7
100
%
0
367.0505
<==measured mass of [M+Na]+
predicted mass of [M+Na]+ is 367.0511
368.0524
365.1538
369.0481
371.2241
363.1241
362 363 364 365 366 367 368 369 370 371 372 373 374 375 376 377 378 379 380
m/z
S
H
H3C
N
N
O
O


Alan Kiste 46-B Electrospray {with Na+ added}
ak46B 8 (1.609) Cn (Cen,5, 50.00, Ht); Sb (15,40.00 ); Sm (SG, 1x5.00); Cm (2:8)
Magnet ES+
272
100
%
0
195.1
227.1
367.0
261.1
305.2
408.1
m/z
100 200 300 400 500 600 700 800 900 1000 1100 1200 1300 1400 1500 1600 1700
S
H
H3C
N
N
O
O


H1C
H1A
C1
O1
H1B
N1
H5
C2
C3
C5
O2
N4
S6
H8B
C8
H8A
C7
H7A
H7B

Space Group: Monoclinic P2₁/c

p21c.res

```
TITL p21c in P2(1)/c
CELL 0.71073   6.6160  13.9550   8.0050  90.000  92.202  90.000
ZERR    2.00   2.0000   0.0035   0.0074   0.000   0.014   0.000
LATT  1
SYMM -X, 0.5+Y, 0.5-Z
SFAC C H N O S
UNIT 24 32 8 8 4
TEMP -120

L.S. 4
BOND
FMAP 2
PLAN 5

WGHT    0.119400
FVAR       0.26916
S6    5    0.933504    0.475736    0.201924    11.00000    0.04194    0.02089 =
          0.02175   -0.00561    0.01168   -0.01046
N1    3    0.861982    0.289283    0.085055    11.00000    0.01874    0.01795 =
          0.01217   -0.00014    0.00764    0.00093
N4    3    0.596789    0.377448    0.166656    11.00000    0.01549    0.03390 =
          0.02153   -0.00376    0.00312    0.01109
C1    1    1.047402    0.263993    0.006940    11.00000    0.01583    0.02581 =
          0.02227   -0.00455    0.00743    0.00313
AFIX 137
H1A   2    1.102825    0.205389    0.058249    11.00000   -1.50000
H1B   2    1.145371    0.316230    0.022242    11.00000   -1.50000
H1C   2    1.020023    0.253173   -0.112759    11.00000   -1.50000
AFIX   0
C2    1    0.737465    0.226964    0.155645    11.00000    0.02691    0.02091 =
          0.01251   -0.00040   -0.00284   -0.00910
C3    1    0.569051    0.287810    0.226401    11.00000    0.01933    0.03835 =
          0.01355    0.00321   -0.00247   -0.00005
O1    4    0.759427    0.141600    0.170090    11.00000    0.05058    0.01772 =
          0.02292    0.00520   -0.00131   -0.00906
O2    4    0.441438    0.258958    0.316520    11.00000    0.02611    0.07661 =
          0.02707    0.00086    0.01414   -0.01574
C5    1    0.783232    0.386315    0.083158    11.00000    0.03104    0.01294 =
          0.00933    0.00351    0.00618    0.00137
AFIX  13
H5    2    0.757310    0.408480   -0.034516    11.00000   -1.20000
AFIX   0
C7    1    0.730218    0.502108    0.340959    11.00000    0.05491    0.02200 =
          0.01950   -0.00369    0.01411    0.00840
AFIX  23
H7A   2    0.754198    0.469939    0.450154    11.00000   -1.20000
H7B   2    0.719659    0.572003    0.359916    11.00000   -1.20000
AFIX   0
C8    1    0.536347    0.463653    0.252227    11.00000    0.03905    0.03745 =
          0.03026   -0.00132    0.00812    0.02453
AFIX  23
H8A   2    0.432666    0.448900    0.334384    11.00000   -1.20000
H8B   2    0.480215    0.511308    0.171425    11.00000   -1.20000
HKLF 4
REM  p21c in P2(1)/c
REM R1 =  0.1191 for    830 Fo > 4sig(Fo)  and  0.2159 for all   1890 data
REM    101 parameters refined using      0 restraints

END

WGHT      0.1207      0.0000
REM Highest difference peak  0.562,  deepest hole -0.462,  1-sigma level  0.113
```



z

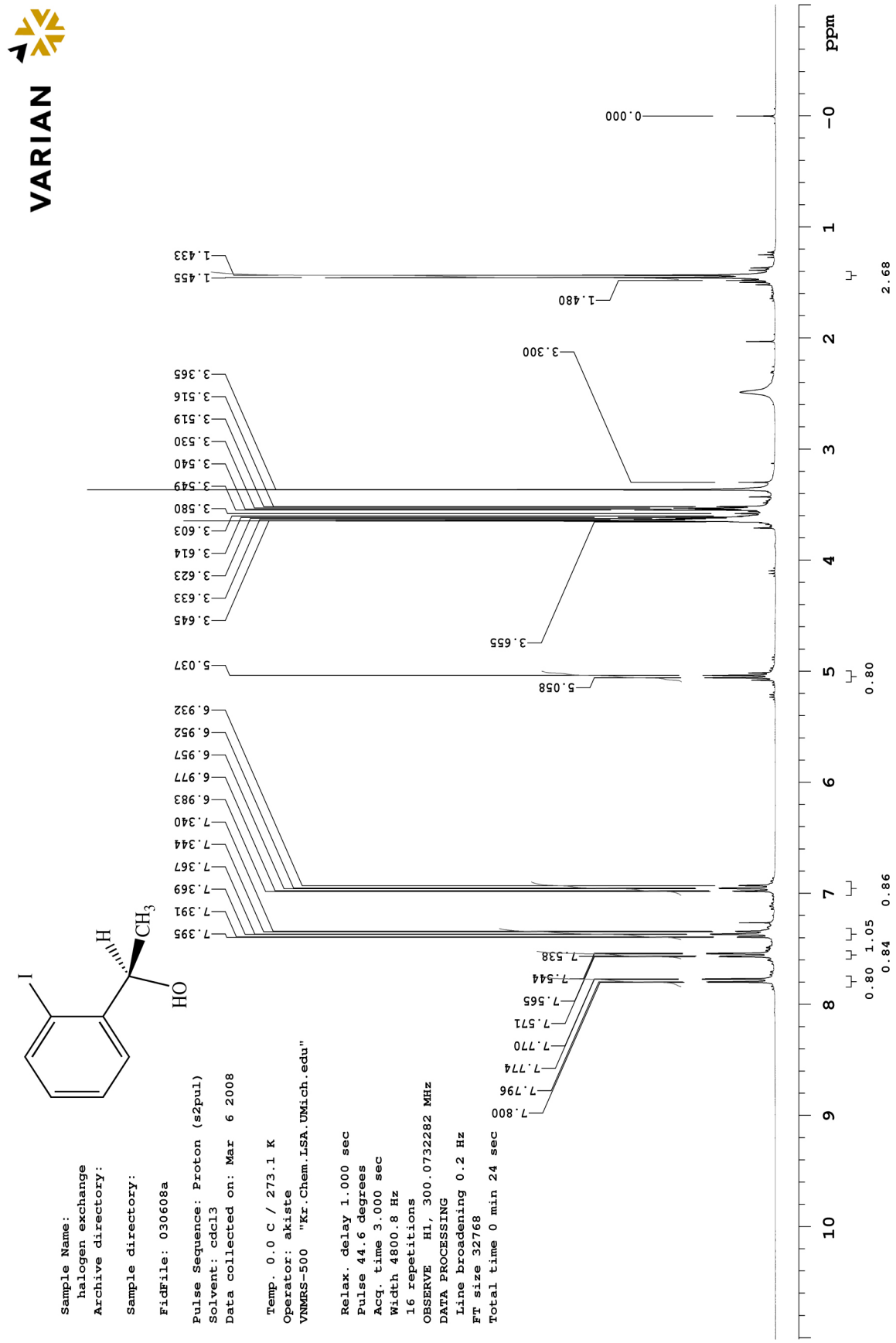
unit cell parameters (a, b, c, α, β, γ)

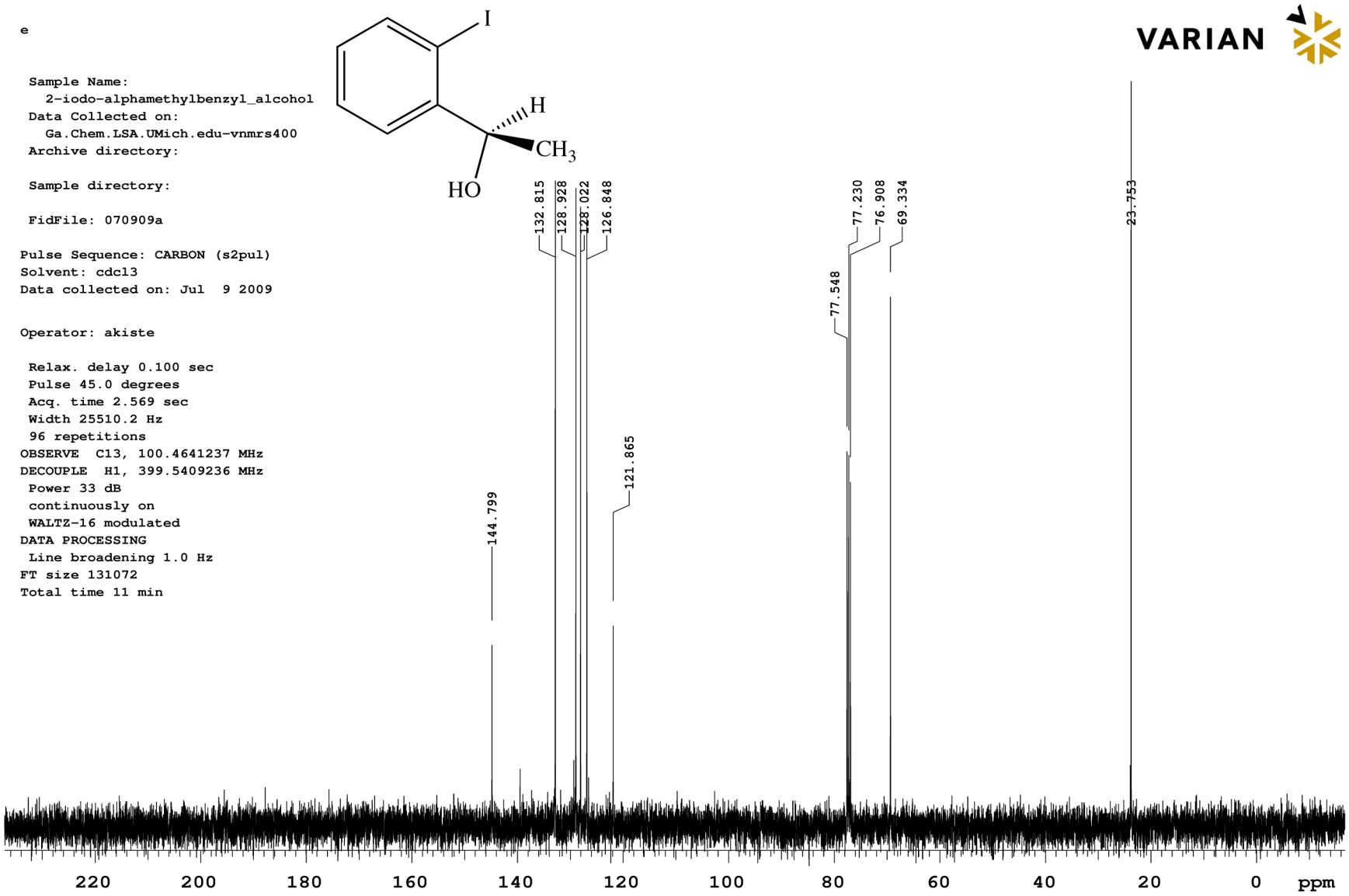
error in cell parameters

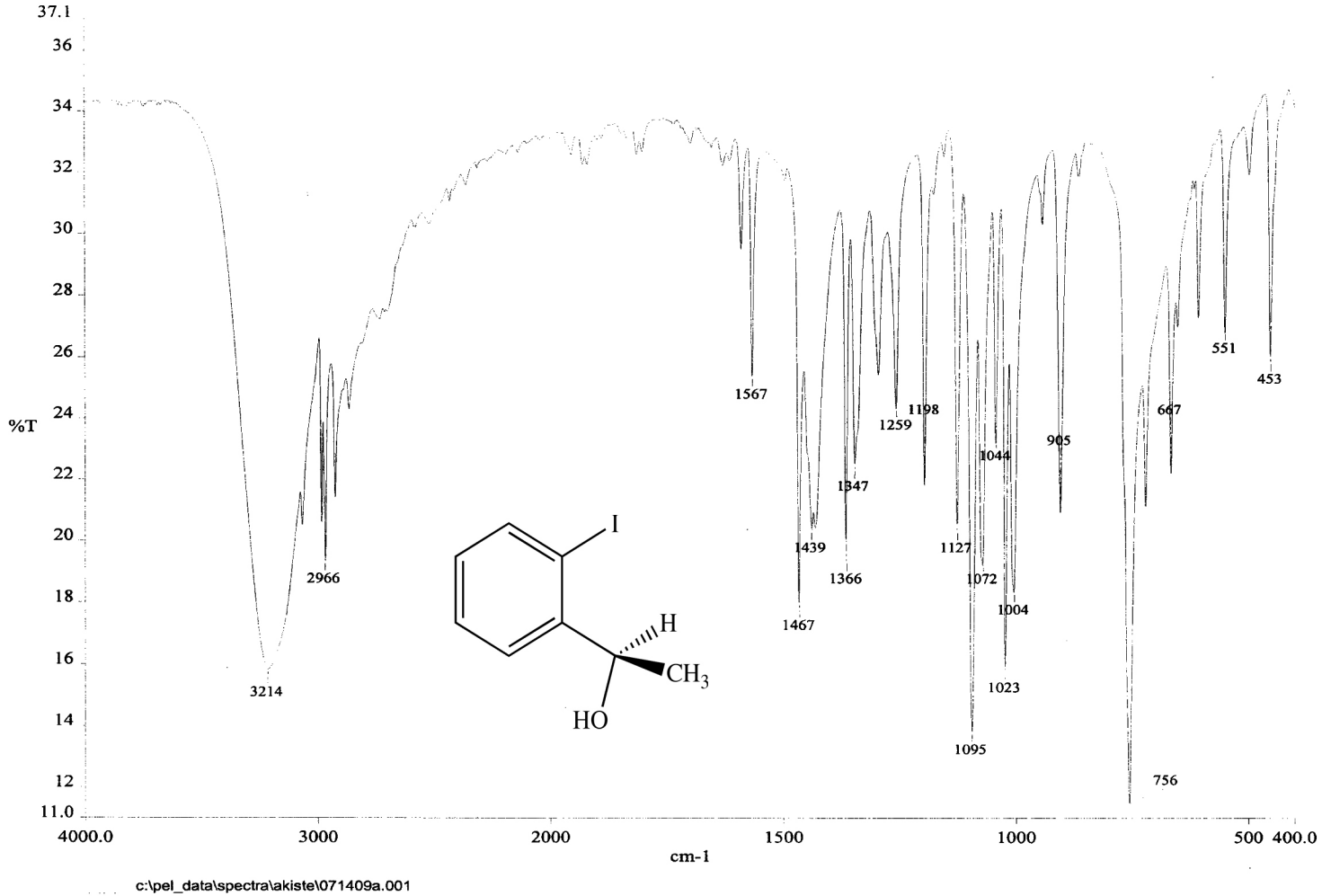
note a-axis is severely twinned

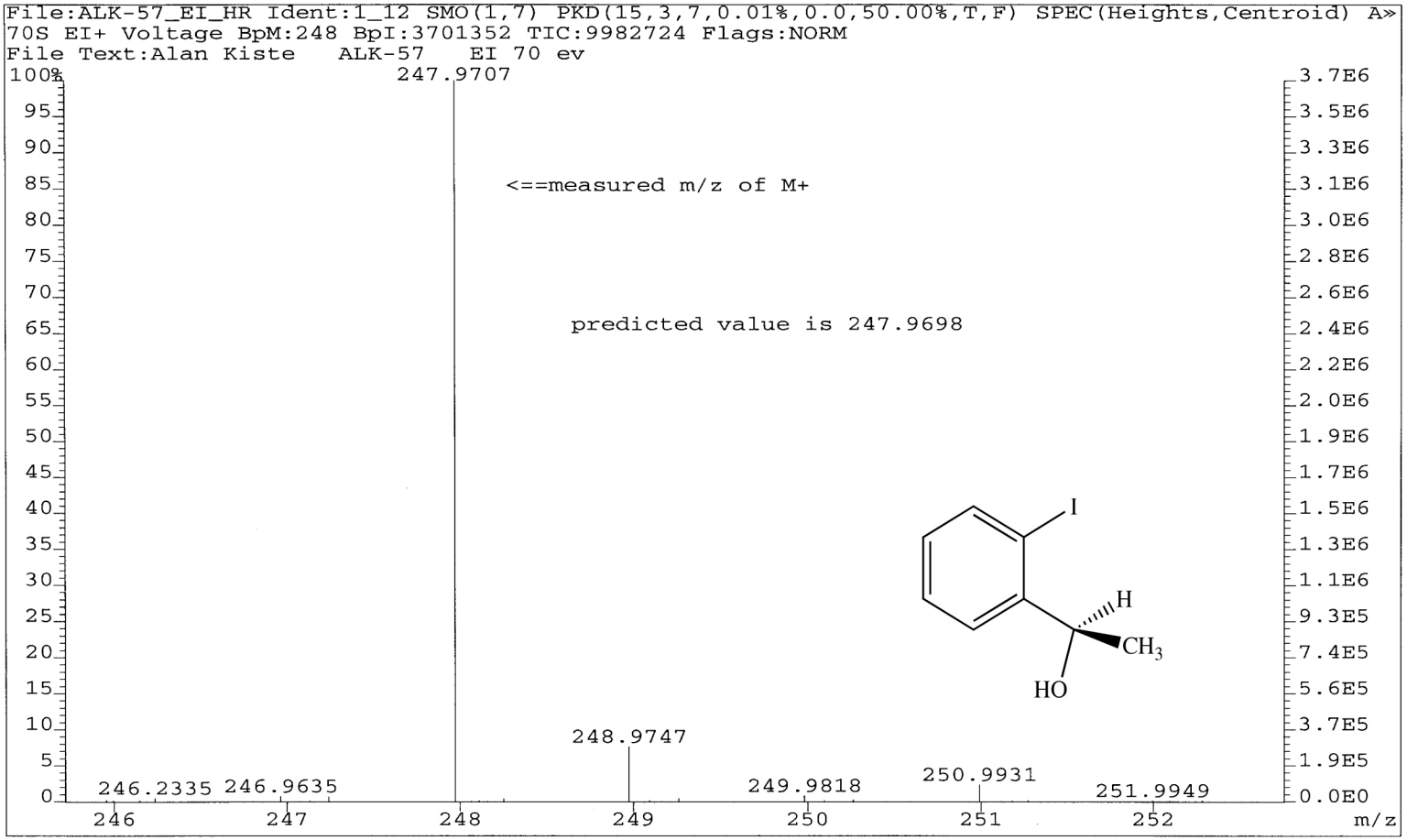
current R₁

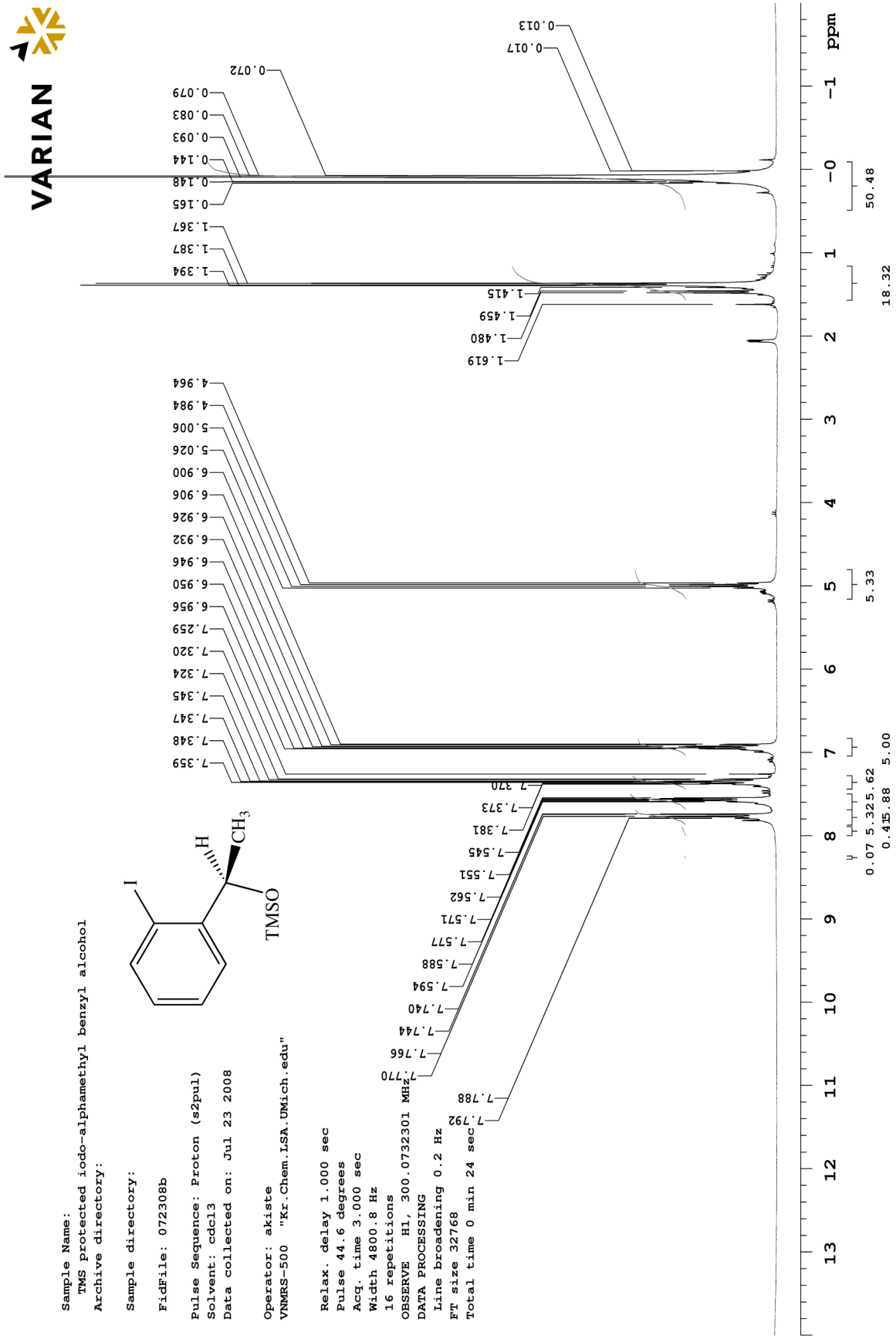
current wR2


VARIAN
Sample Name:
halogen exchange
Archive directory:
Sample directory:
FidFile: 030608a
Pulse Sequence: Proton (s2pul)
Solvent: cdcl3
Data collected on: Mar 6 2008
Temp. 0.0 C / 273.1 K
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Relax. delay 1.000 sec
Pulse 44.6 degrees
Acq. time 3.000 sec
Width 4800.8 Hz
16 repetitions
OBSERVE H1, 300.0732282 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min 24 sec
I
H
CH3
HO
7.800
7.796
7.774
7.770
7.571
7.565
7.544
7.538
7.395
7.391
7.369
7.367
7.344
7.340
6.983
6.977
6.957
6.952
6.932
5.037
5.058
3.655
3.645
3.633
3.623
3.614
3.603
3.580
3.549
3.540
3.530
3.519
3.516
3.365
3.300
1.480
1.455
1.433
0.000
ppm
0.80
1.05
0.84
0.86
0.80
2.68


e
Sample Name:
2-iodo-alphamethylbenzyl_alcohol
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909a
Pulse Sequence: CARBON (s2pul)
Solvent: cdcl3
Data collected on: Jul 9 2009
Operator: akiste
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
96 repetitions
OBSERVE C13, 100.4641237 MHz
DECOUPLE H1, 399.5409236 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 11 min
I
H
CH3
HO
VARIAN
144.799
132.815
128.928
128.022
126.848
121.865
77.548
77.230
76.908
69.334
23.753
220
200
180
160
140
120
100
80
60
40
20
0
ppm


37.1
36
34
32
30
28
26
24
22
20
18
16
14
12
11.0
%T
4000.0
3000
2000
1500
1000
500
400.0
cm-1
3214
2966
1567
1467
1439
1366
1347
1259
1198
1127
1095
1072
1044
1023
1004
905
756
667
551
453
I
H
CH3
HO
c:\pel_data\spectra\akiste\071409a.001


File:ALK-57_EI_HR Ident:1_12 SMO(1,7) PKD(15,3,7,0.01%,0.0,50.00%,T,F) SPEC(Heights,Centroid) A»
70S EI+ Voltage BpM:248 BpI:3701352 TIC:9982724 Flags:NORM
File Text:Alan Kiste ALK-57 EI 70 ev
247.9707
<==measured m/z of M+
predicted value is 247.9698
248.9747
246.2335
246.9635
249.9818
250.9931
251.9949
I
H
CH3
HO
m/z


VARIAN
Sample Name:
TMS protected iodo-alphamethyl benzyl alcohol
Archive directory:
Sample directory:
FidFile: 072308b
Pulse Sequence: Proton (s2pul)
Solvent: cdcl3
Data collected on: Jul 23 2008
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Relax. delay 1.000 sec
Pulse 44.6 degrees
Acq. time 3.000 sec
Width 4800.8 Hz
16 repetitions
OBSERVE H1, 300.0732301 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min 24 sec
I
H
CH3
TMSO
0.013
0.017
0.072
0.079
0.083
0.093
0.144
0.148
0.165
1.367
1.387
1.394
1.415
1.459
1.480
1.619
4.964
4.984
5.006
5.026
6.900
6.906
6.926
6.932
6.946
6.950
6.956
7.259
7.320
7.324
7.345
7.347
7.348
7.359
7.370
7.373
7.381
7.545
7.551
7.562
7.571
7.577
7.588
7.594
7.740
7.744
7.766
7.770
7.788
7.792
ppm
50.48
18.32
5.33
0.07 5.32 5.62
0.41 5.88 5.00

Std Carbon experiment

Sample Name:
TMS protected iodo-alphamethyl benzyl alcohol
Archive directory:

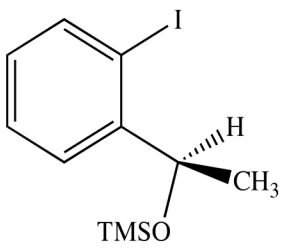
Sample directory:

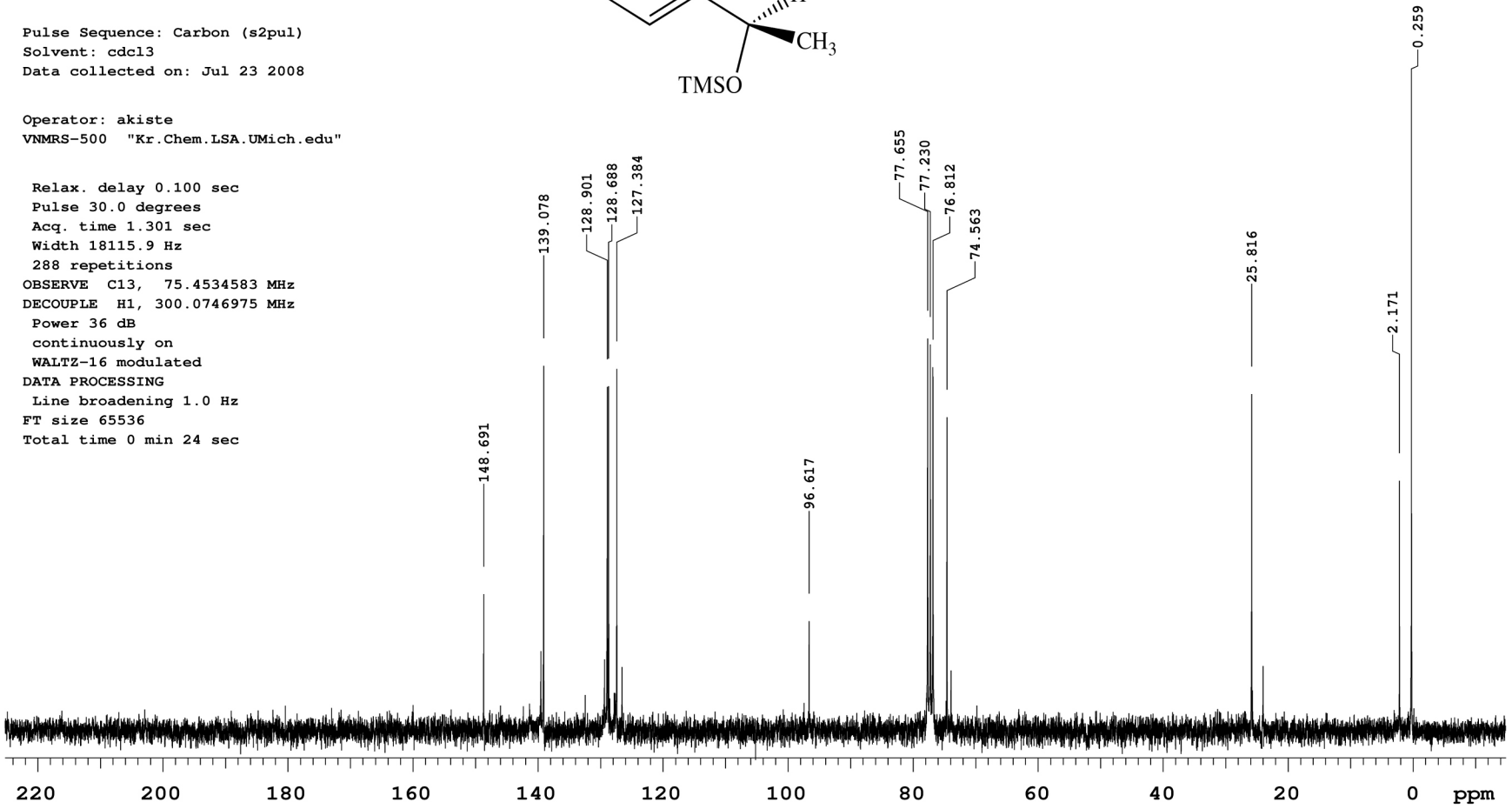
FidFile: 072308a

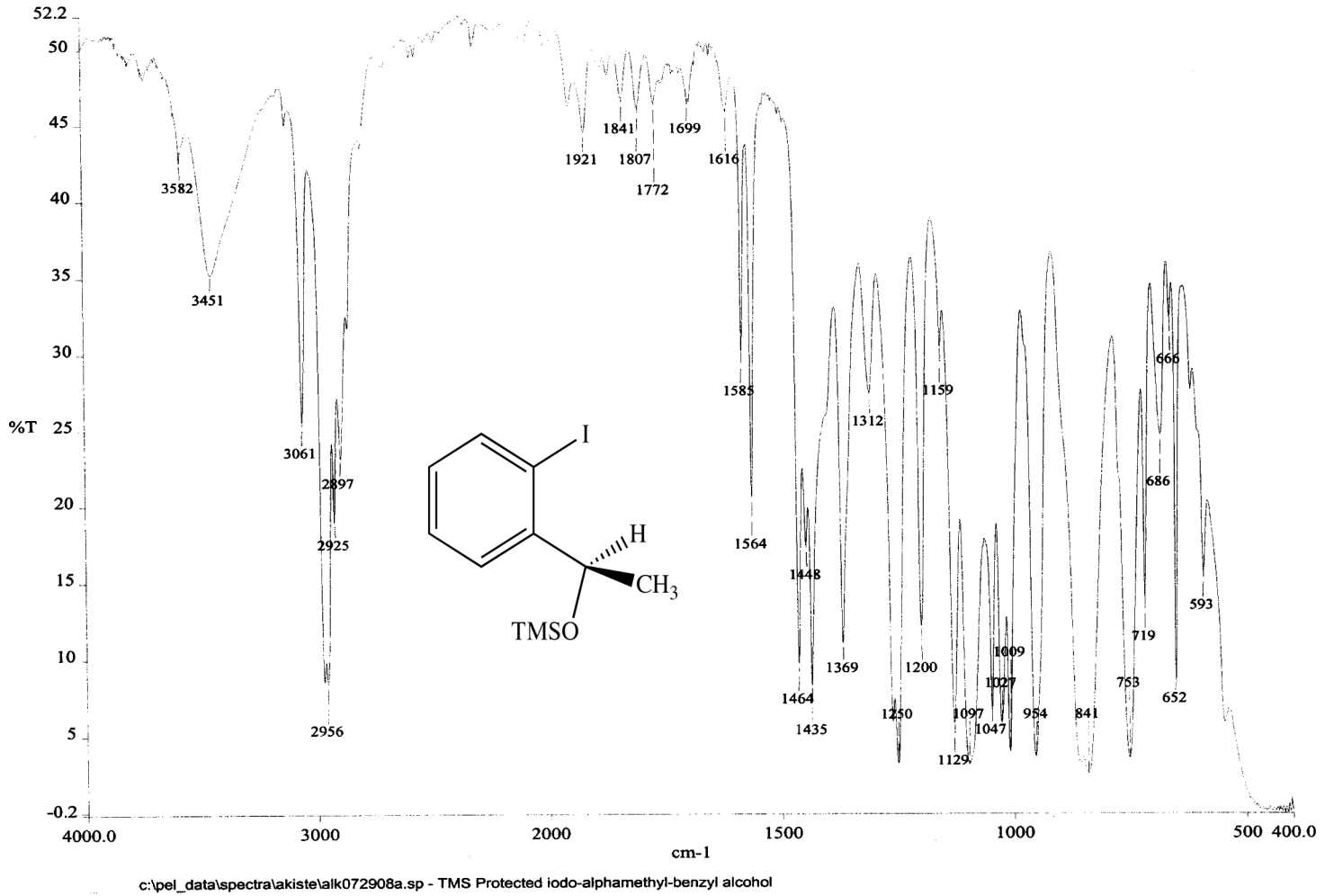
Pulse Sequence: Carbon (s2pul)
Solvent: cdcl3
Data collected on: Jul 23 2008

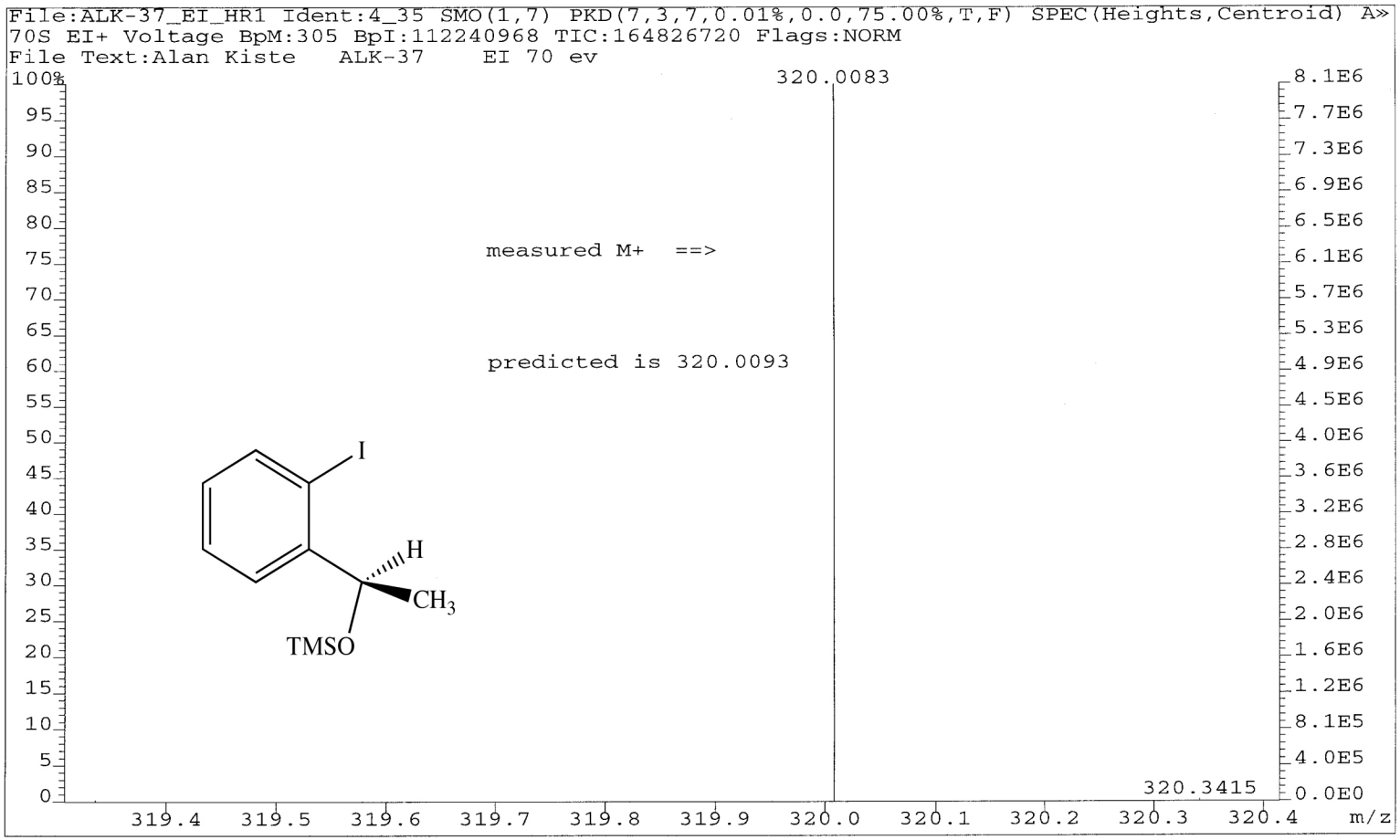
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"

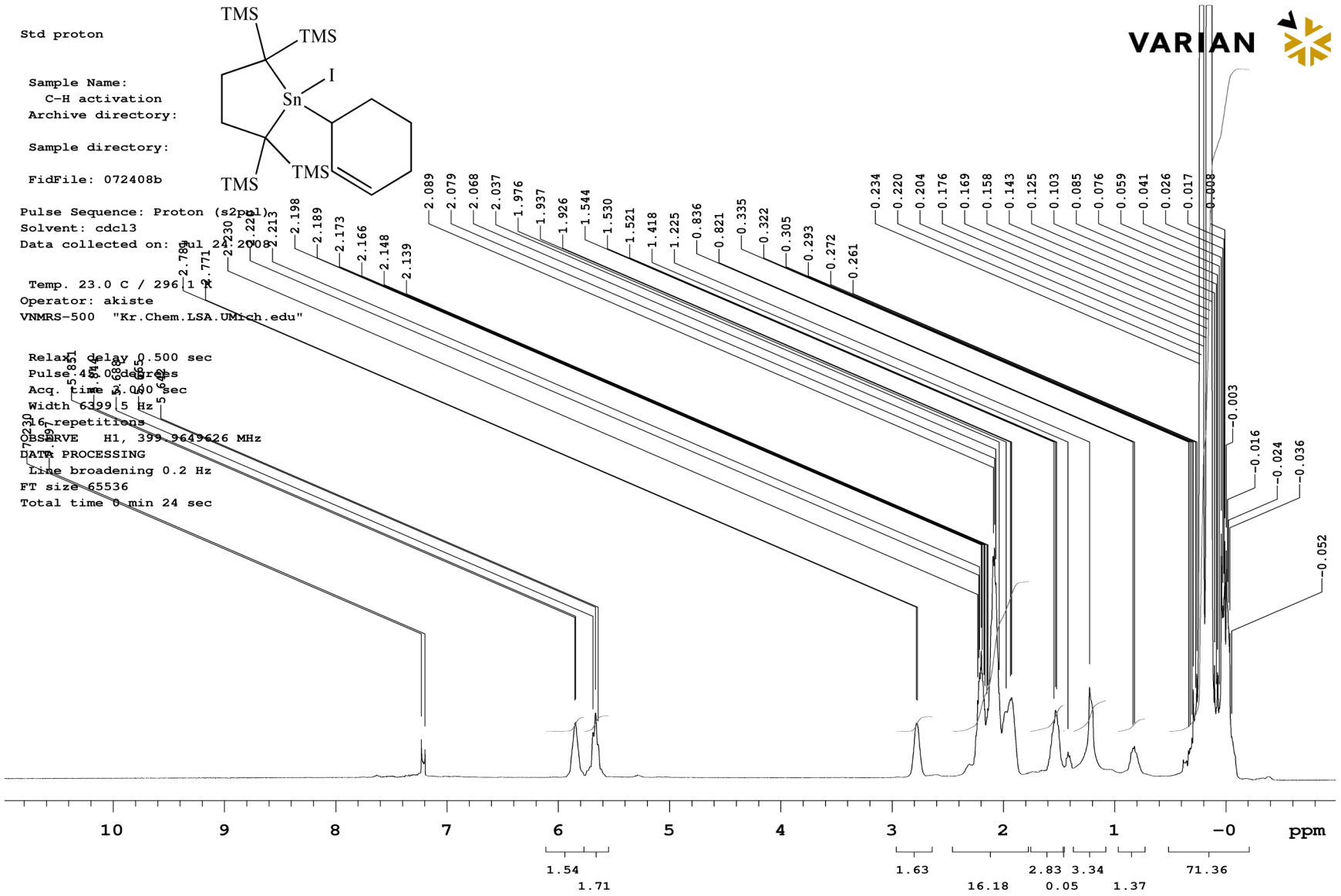
Relax. delay 0.100 sec
Pulse 30.0 degrees
Acq. time 1.301 sec
Width 18115.9 Hz
288 repetitions
OBSERVE C13, 75.4534583 MHz
DECOUPLE H1, 300.0746975 MHz
Power 36 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 0 min 24 sec




52.2
50
45
40
35
30
%T 25
20
15
10
5
-0.2
4000.0
3000
2000
1500
1000
500 400.0
cm-1
3582
3451
3061
2897
2925
2956
1921
1841
1807
1772
1699
1616
1585
1564
1448
1464
1435
1369
1312
1250
1200
1159
1129
1097
1047
1027
1009
954
841
753
719
686
666
652
593
I
H
CH3
TMSO
c:\pel_data\spectra\akiste\alk072908a.sp - TMS Protected iodo-alphamethyl-benzyl alcohol


File:ALK-37_EI_HR1 Ident:4_35 SMO(1,7) PKD(7,3,7,0.01%,0.0,75.00%,T,F) SPEC(Heights,Centroid) A»
70S EI+ Voltage BpM:305 BpI:112240968 TIC:164826720 Flags:NORM
File Text:Alan Kiste ALK-37 EI 70 ev
320.0083
measured M+ ==>
predicted is 320.0093
320.3415
I
H
CH3
TMSO
m/z


Std proton
Sample Name:
C-H activation
Archive directory:
Sample directory:
FidFile: 072408b
Pulse Sequence: Proton (s2pul)
Solvent: cdcl3
Data collected on: Jul 24 2008
Temp. 23.0 C / 296.1 K
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"
Relax. delay 0.500 sec
Pulse 45.0 degrees
Acq. time 3.000 sec
Width 6399.5 Hz
16 repetitions
OBSERVE H1, 399.9649626 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 0 min 24 sec
TMS
TMS
I
Sn
TMS
TMS
VARIAN
ppm
1.54
1.71
1.63
16.18
2.83
0.05
3.34
1.37
71.36

Std Carbon

VARIAN

Sample Name:
C-H activation
Archive directory:

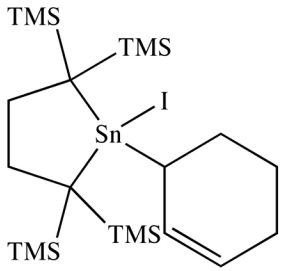
Sample directory:

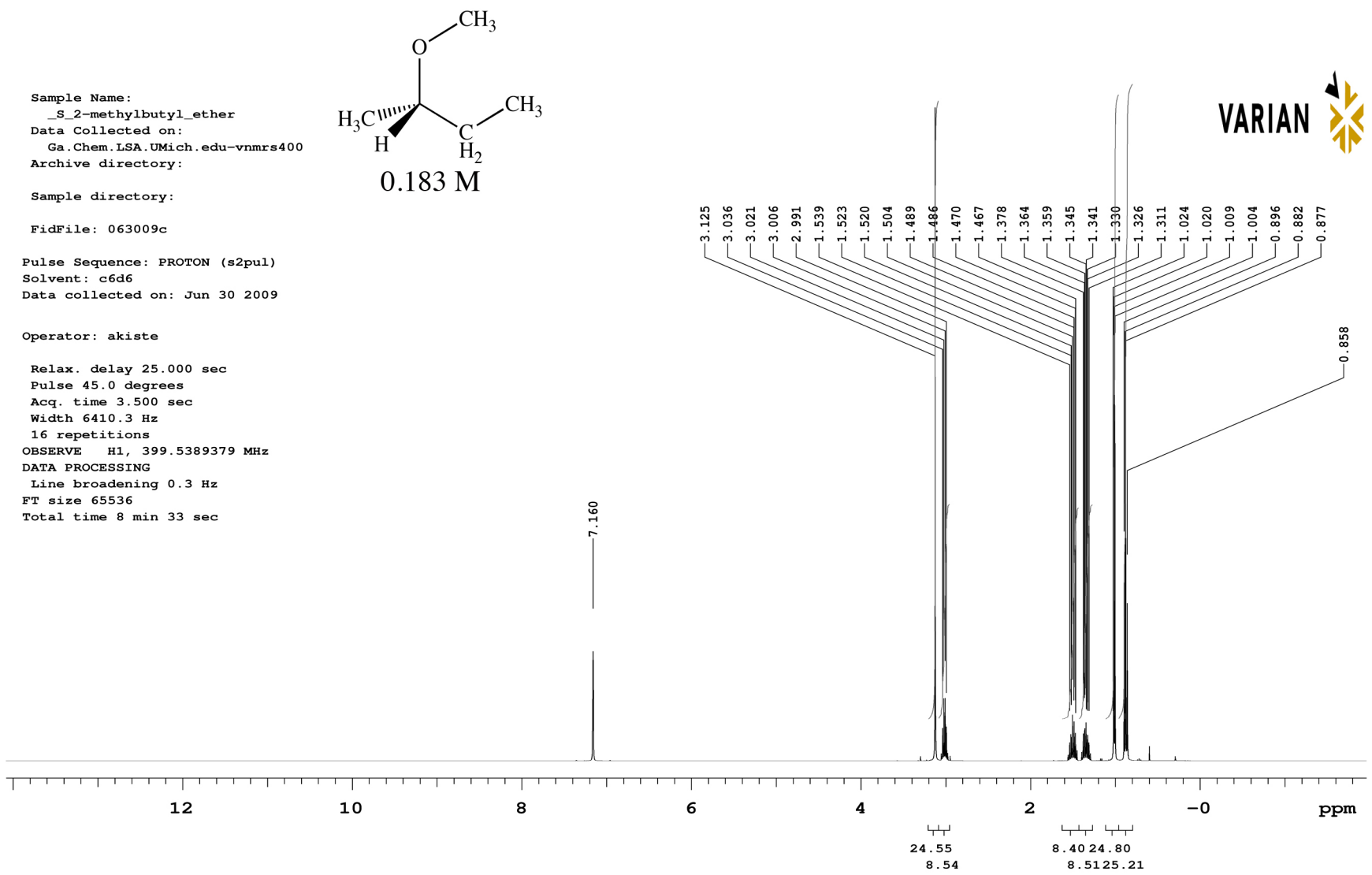
FidFile: 072408a

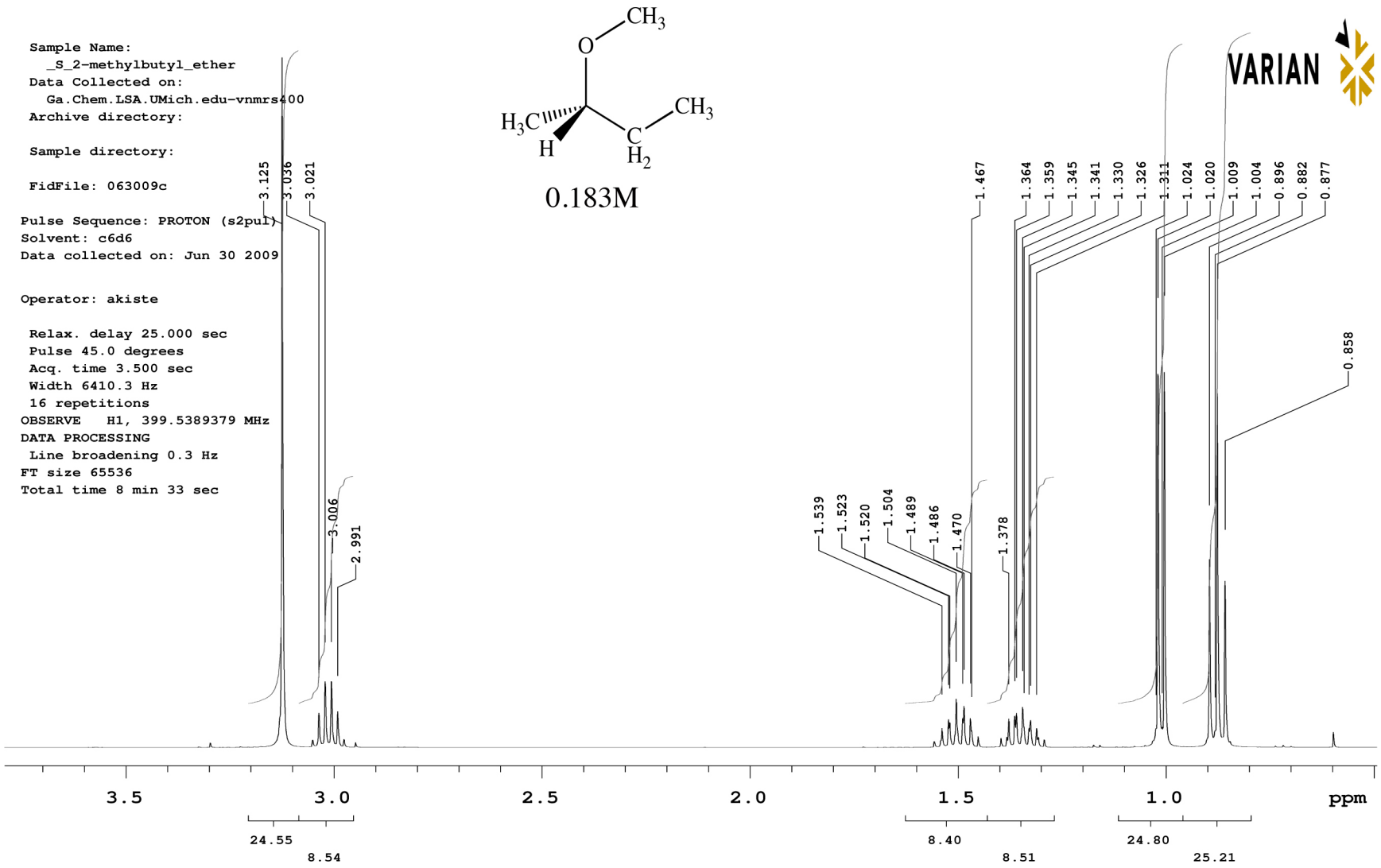
Pulse Sequence: Carbon (s2pul)
Solvent: cdcl3
Data collected on: Jul 24 2008

Temp. 23.0 C / 296.1 K
Operator: akiste
VNMRS-500 "Kr.Chem.LSA.UMich.edu"

Relax. delay 0.100 sec
Pulse 30.0 degrees
Acq. time 1.300 sec
Width 24140.0 Hz
272 repetitions
OBSERVE C13, 100.5712439 MHz
DECOUPLE H1, 399.9669644 MHz
Power 39 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.8 Hz
FT size 65536
Total time 0 min 24 sec




Sample Name:
_S_2-methylbutyl_ether
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 063009c
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jun 30 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.5389379 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 33 sec
0.183 M
VARIAN
3.125
3.036
3.021
3.006
2.991
1.539
1.523
1.520
1.504
1.489
1.486
1.470
1.467
1.378
1.364
1.359
1.345
1.341
1.330
1.326
1.311
1.024
1.020
1.009
1.004
0.896
0.882
0.877
0.858
7.160
12
10
8
6
4
2
−0
ppm
24.55
8.54
8.40
8.51
24.80
25.21


Sample Name:
_S_2-methylbutyl_ether
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 063009c
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jun 30 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.5389379 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 33 sec
0.183M
VARIAN
3.125
3.036
3.021
3.006
2.991
1.539
1.523
1.520
1.504
1.489
1.486
1.470
1.467
1.378
1.364
1.359
1.345
1.341
1.330
1.326
1.311
1.024
1.020
1.009
1.004
0.896
0.882
0.877
0.858
3.5
3.0
2.5
2.0
1.5
1.0
ppm
24.55
8.54
8.40
8.51
24.80
25.21

Probe tuneing parameter

Sample Name:
S-2-methylbutylether
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:

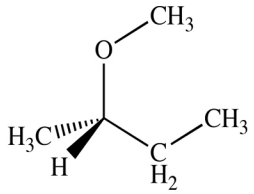
Sample directory:

FidFile: 070109b

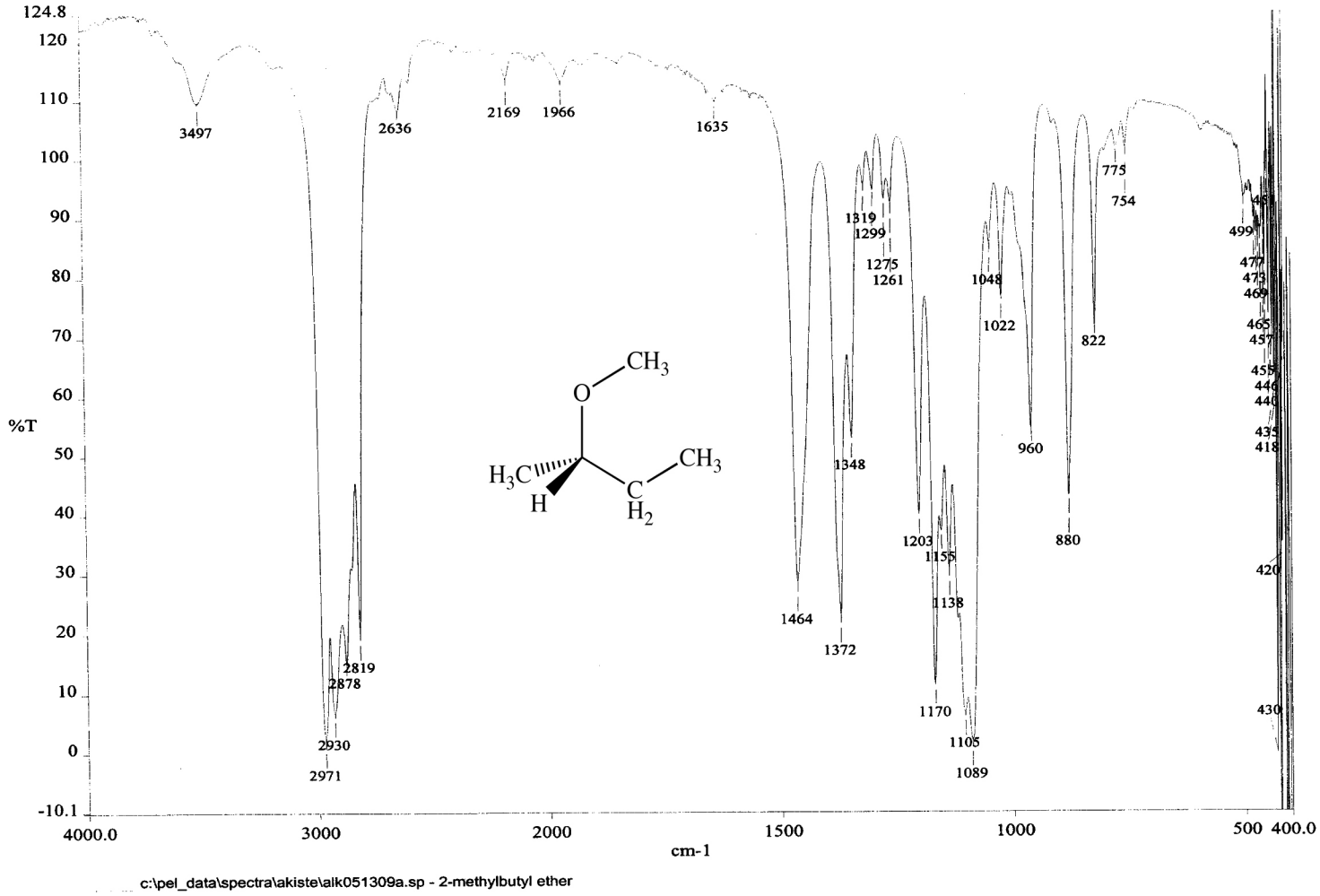
Pulse Sequence: CARBON (s2pul)
Solvent: c6d6
Data collected on: Jul 1 2009

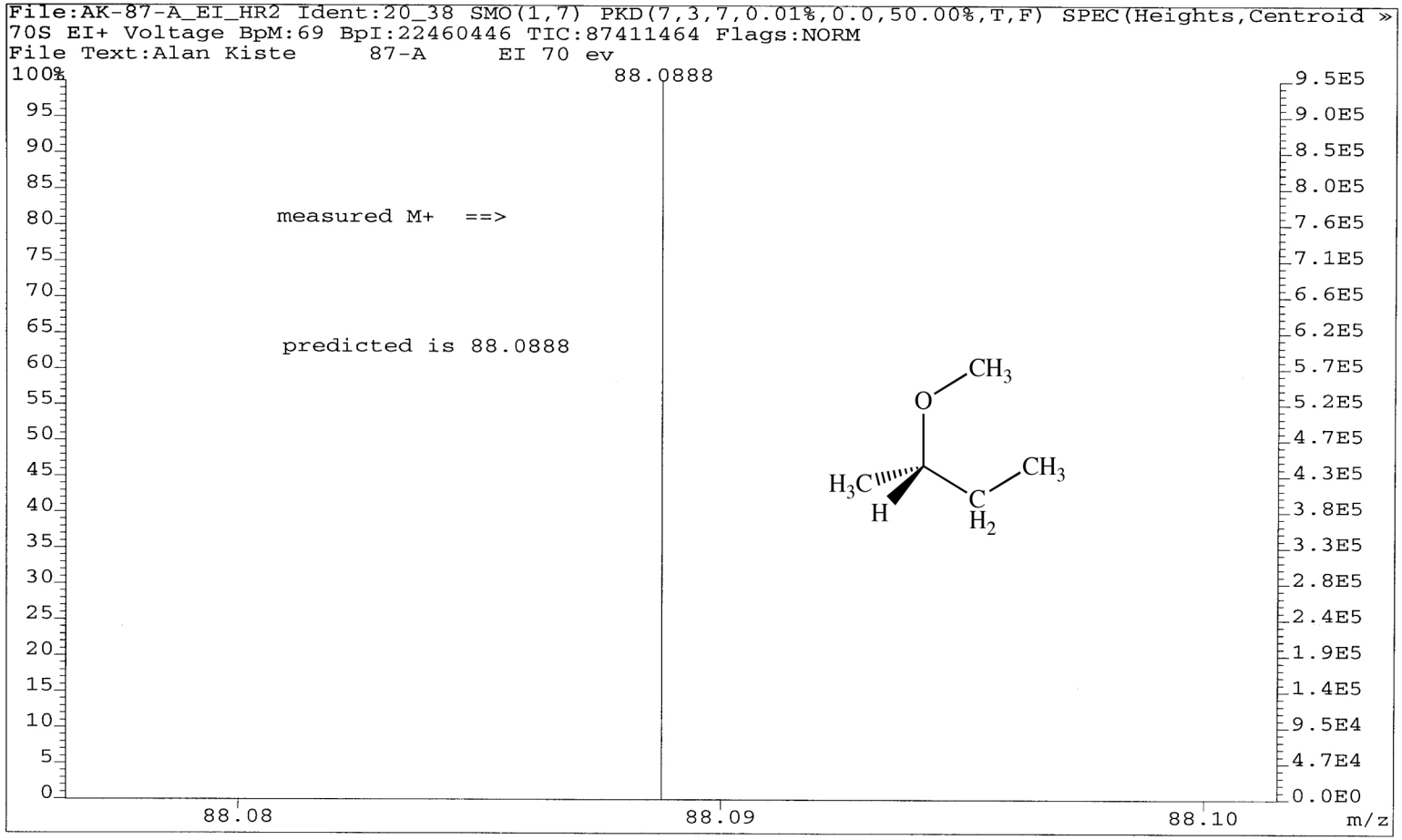
Operator: akiste

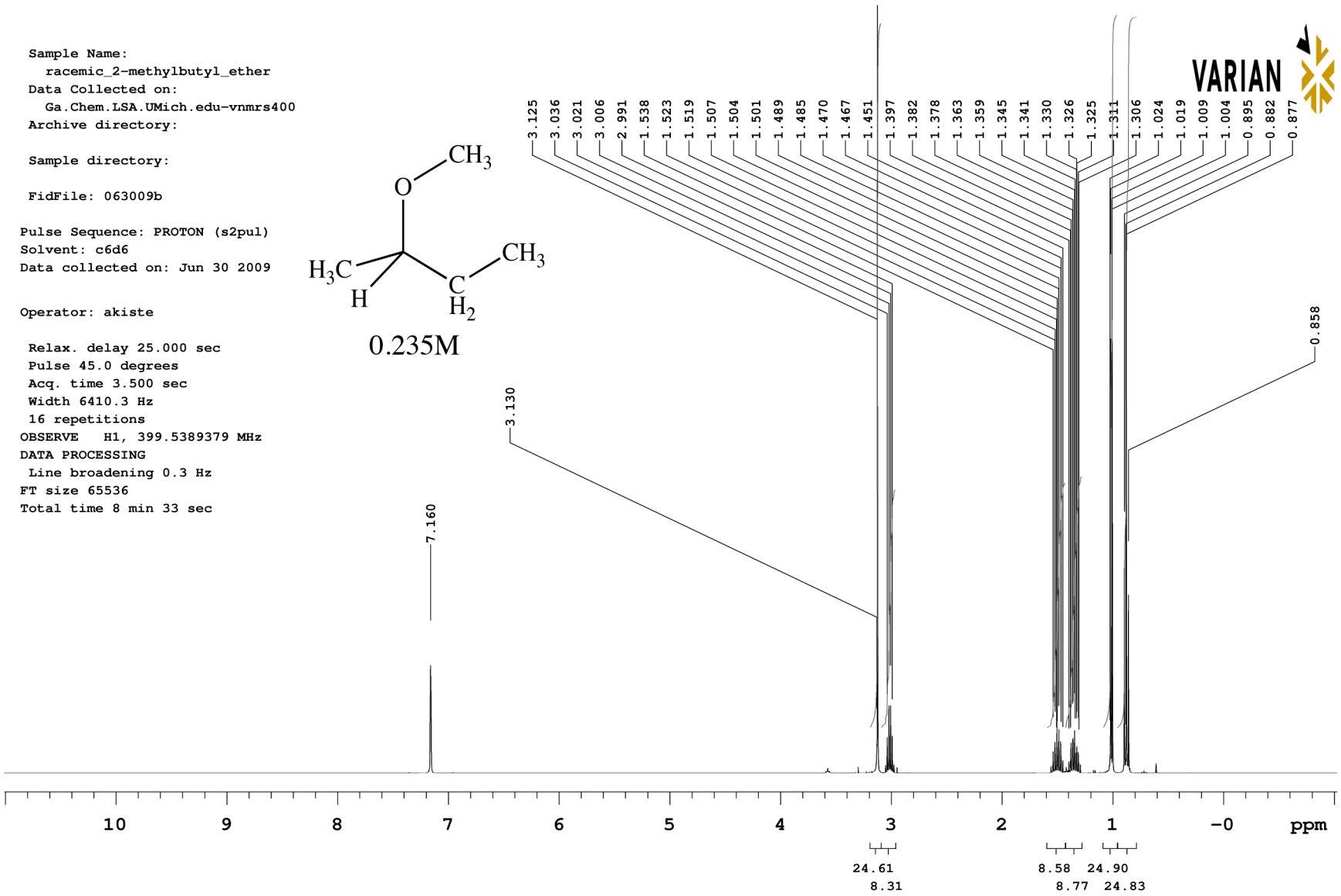
Relax. delay 0.100 sec
Pulse 45.0 degrees
Acq. time 2.569 sec
Width 25510.2 Hz
80 repetitions
OBSERVE C13, 100.4640704 MHz
DECOUPLE H1, 399.5409595 MHz
Power 33 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 11 min

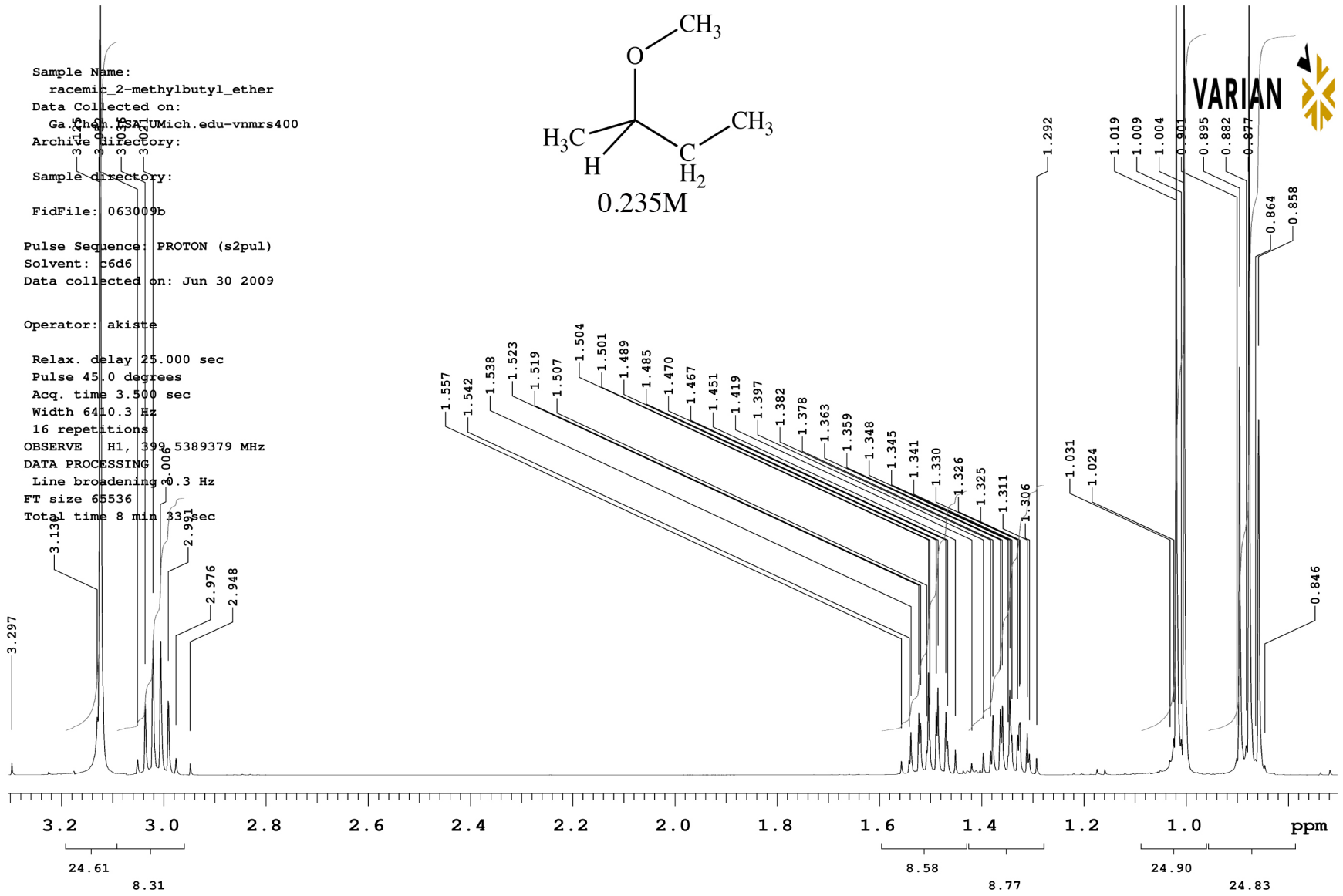



0.183M

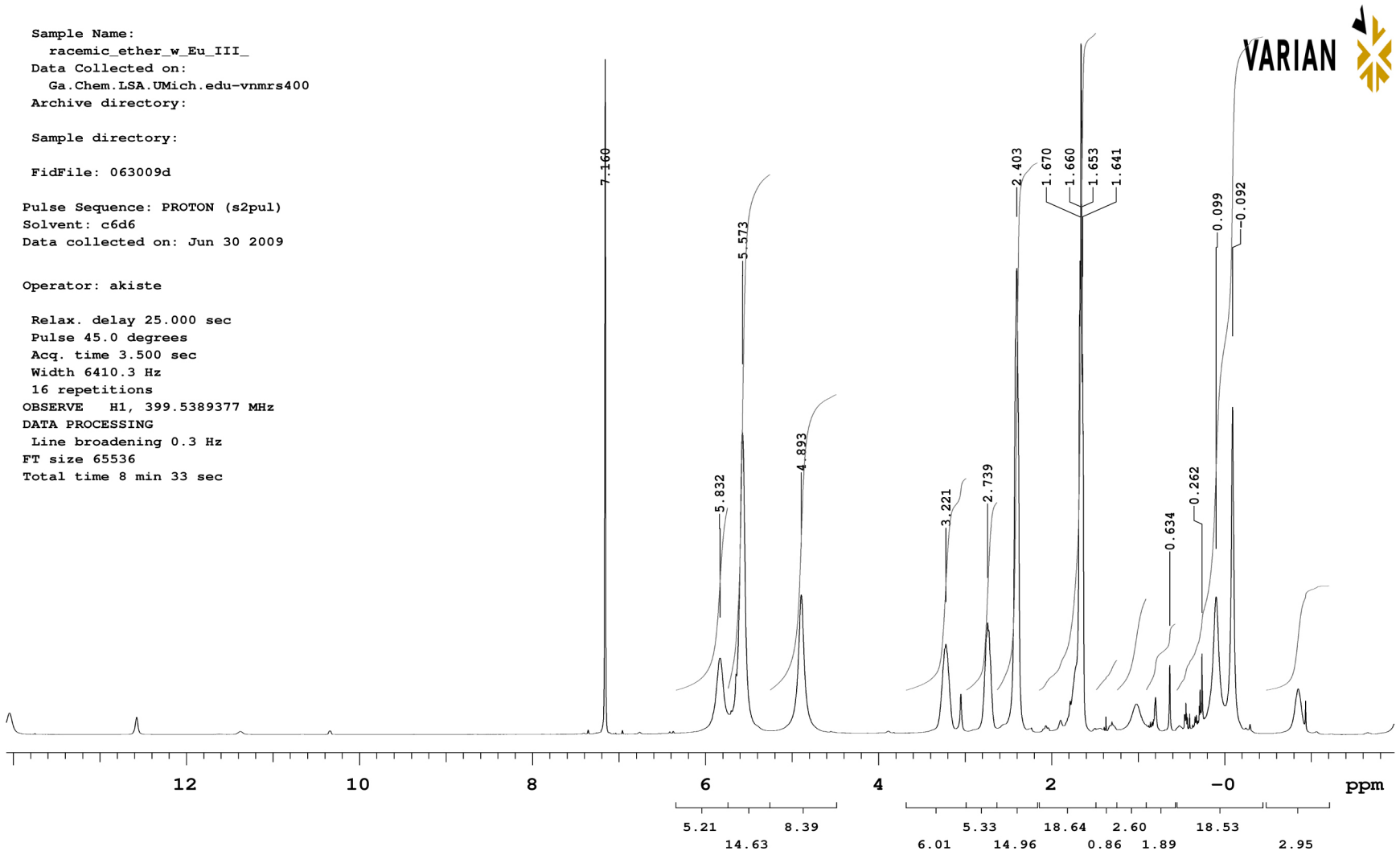

124.8
120
110
100
90
80
70
60
50
40
30
20
10
0
-10.1
%T
4000.0
3000
2000
1500
1000
500
400.0
cm-1
3497
2636
2169
1966
1635
1464
1372
1348
1319
1299
1275
1261
1203
1155
1138
1170
1105
1089
1048
1022
960
880
822
775
754
499
477
473
469
465
457
455
446
440
435
418
420
430
2971
2930
2878
2819
O
CH3
H3C
H
C
H2
CH3
c:\pel_data\spectra\akiste\alk051309a.sp - 2-methylbutyl ether


File:AK-87-A_EI_HR2 Ident:20_38 SMO(1,7) PKD(7,3,7,0.01%,0.0,50.00%,T,F) SPEC(Heights,Centroid »
70S EI+ Voltage BpM:69 BpI:22460446 TIC:87411464 Flags:NORM
File Text:Alan Kiste 87-A EI 70 ev
88.0888
measured M+ ==>
predicted is 88.0888
100%
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
9.5E5
9.0E5
8.5E5
8.0E5
7.6E5
7.1E5
6.6E5
6.2E5
5.7E5
5.2E5
4.7E5
4.3E5
3.8E5
3.3E5
2.8E5
2.4E5
1.9E5
1.4E5
9.5E4
4.7E4
0.0E0
88.08
88.09
88.10
m/z
O
CH3
H3C
H
C
H2
CH3

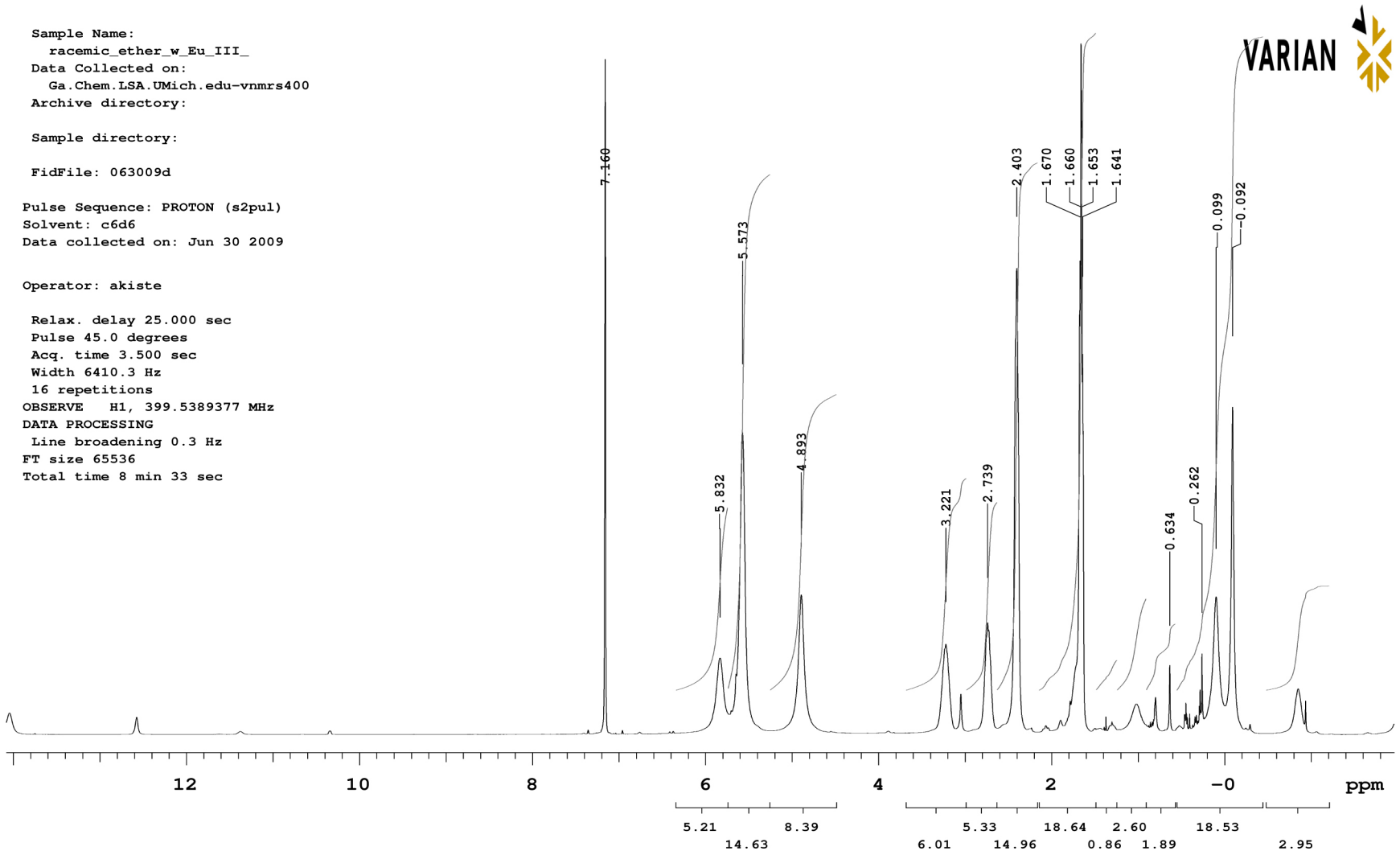

Sample Name:
racemic_2-methylbutyl_ether
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 063009b
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jun 30 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.5389379 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 33 sec
0.235M
VARIAN
3.125
3.036
3.021
3.006
2.991
1.538
1.523
1.519
1.507
1.504
1.501
1.489
1.485
1.470
1.467
1.451
1.397
1.382
1.378
1.363
1.359
1.345
1.341
1.330
1.326
1.325
1.311
1.306
1.024
1.019
1.009
1.004
0.895
0.882
0.877
0.858
3.130
7.160
10
9
8
7
6
5
4
3
2
1
−0
ppm
24.61
8.31
8.58
8.77
24.90
24.83


Sample Name:
racemic_2-methylbutyl_ether
Data Collected on:
Ga.chem.ISA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 063009b
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jun 30 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 3.500 sec
Width 6410.3 Hz
16 repetitions
OBSERVE H1, 399.5389379 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 33 sec
0.235M
VARIAN
3.297
3.131
2.991
2.976
2.948
1.557
1.542
1.538
1.523
1.519
1.507
1.504
1.501
1.489
1.485
1.470
1.467
1.451
1.419
1.397
1.382
1.378
1.363
1.359
1.348
1.345
1.341
1.330
1.326
1.325
1.311
1.306
1.292
1.031
1.024
1.019
1.009
1.004
0.901
0.895
0.882
0.877
0.864
0.858
0.846
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
ppm
24.61
8.31
8.58
8.77
24.90
24.83

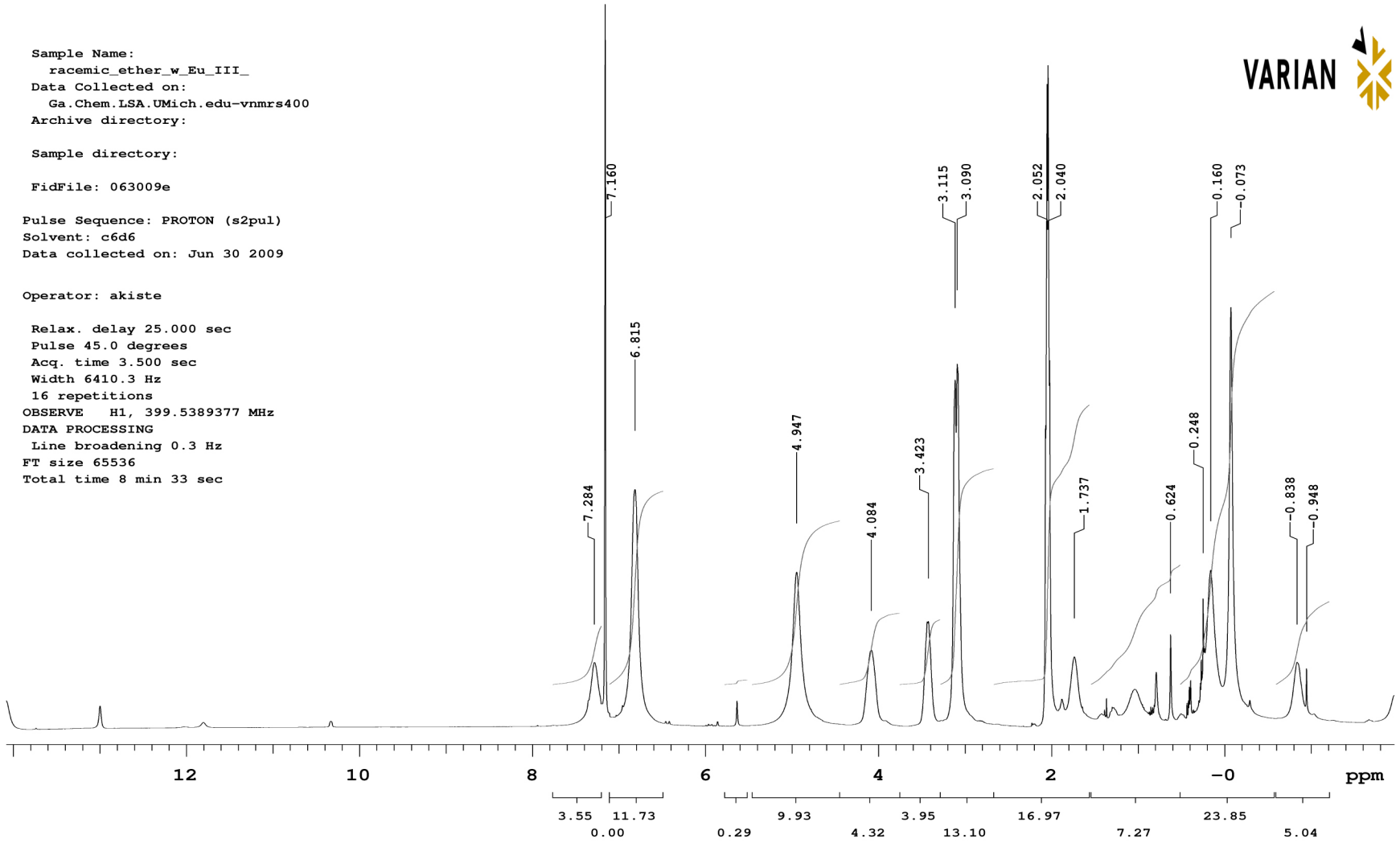
0.235 M ether + 0.0640 M $Eu(hfc)_3$



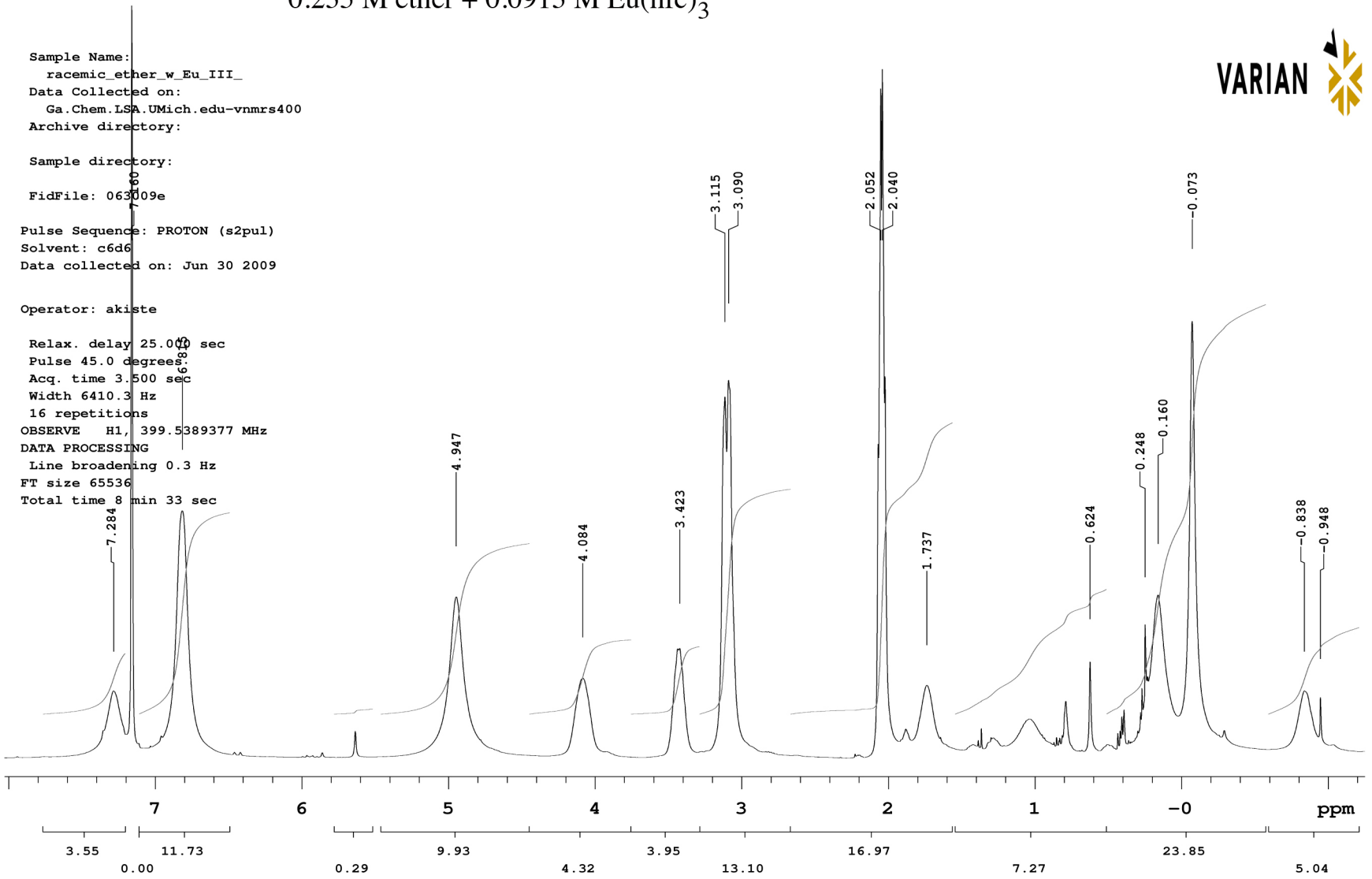
0.235 M ether + 0.0640 M $Eu(hfc)_3$



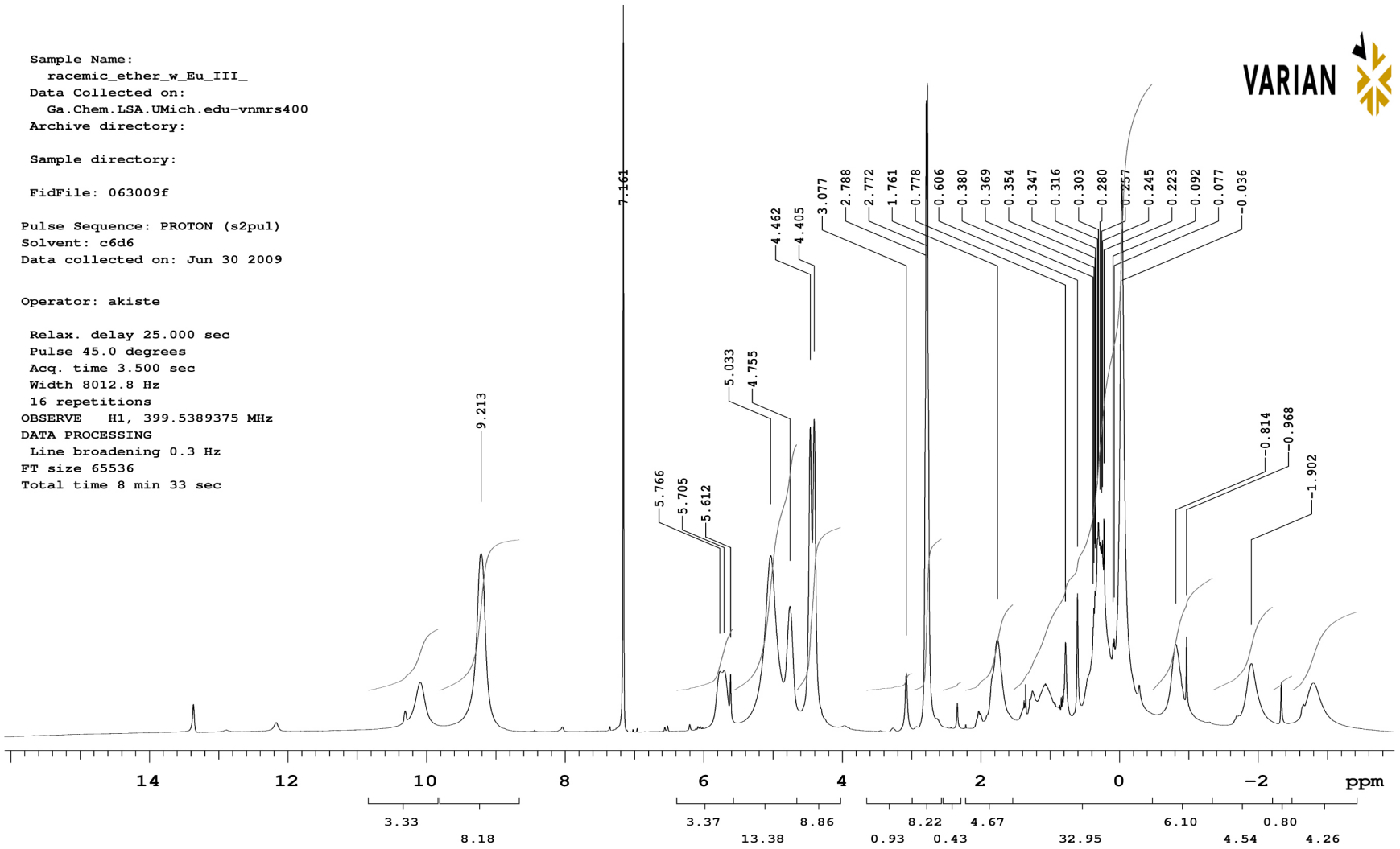
0.235 M ether + 0.0913 M $Eu(hfc)_3$



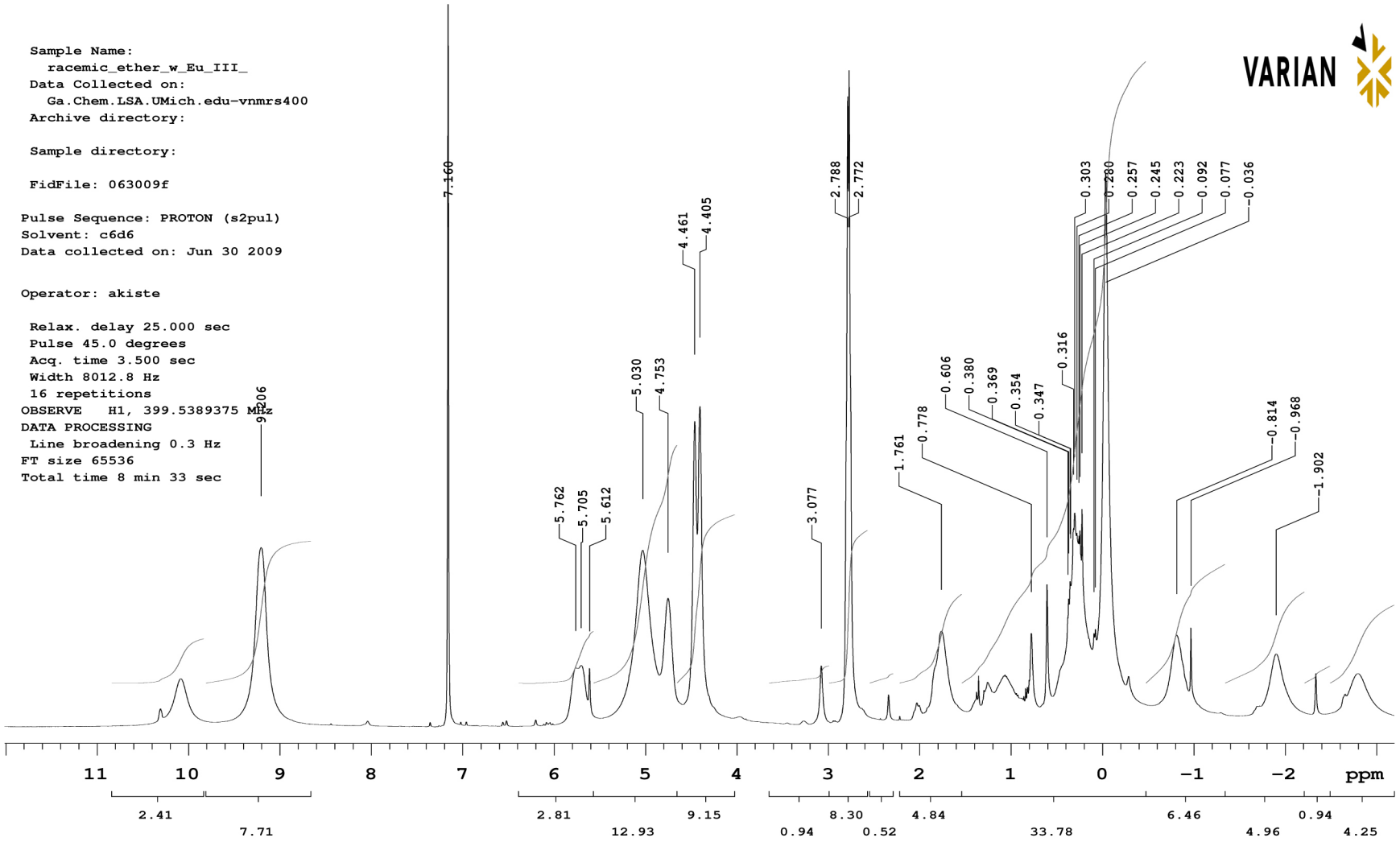
0.235 M ether + 0.0913 M Eu(hfc)$_3$



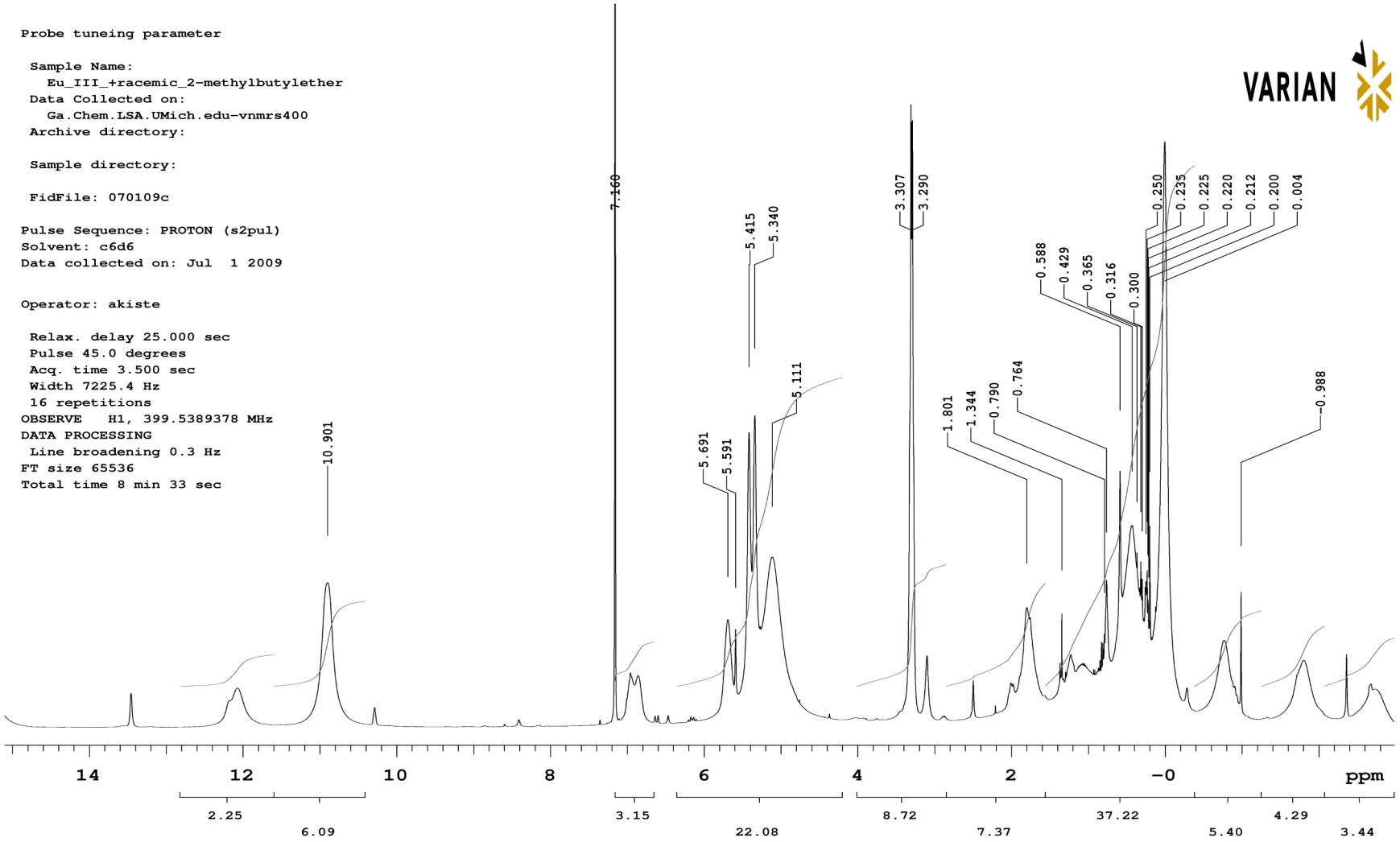
0.235 M ether + 0.142 M $Eu(hfc)_3$



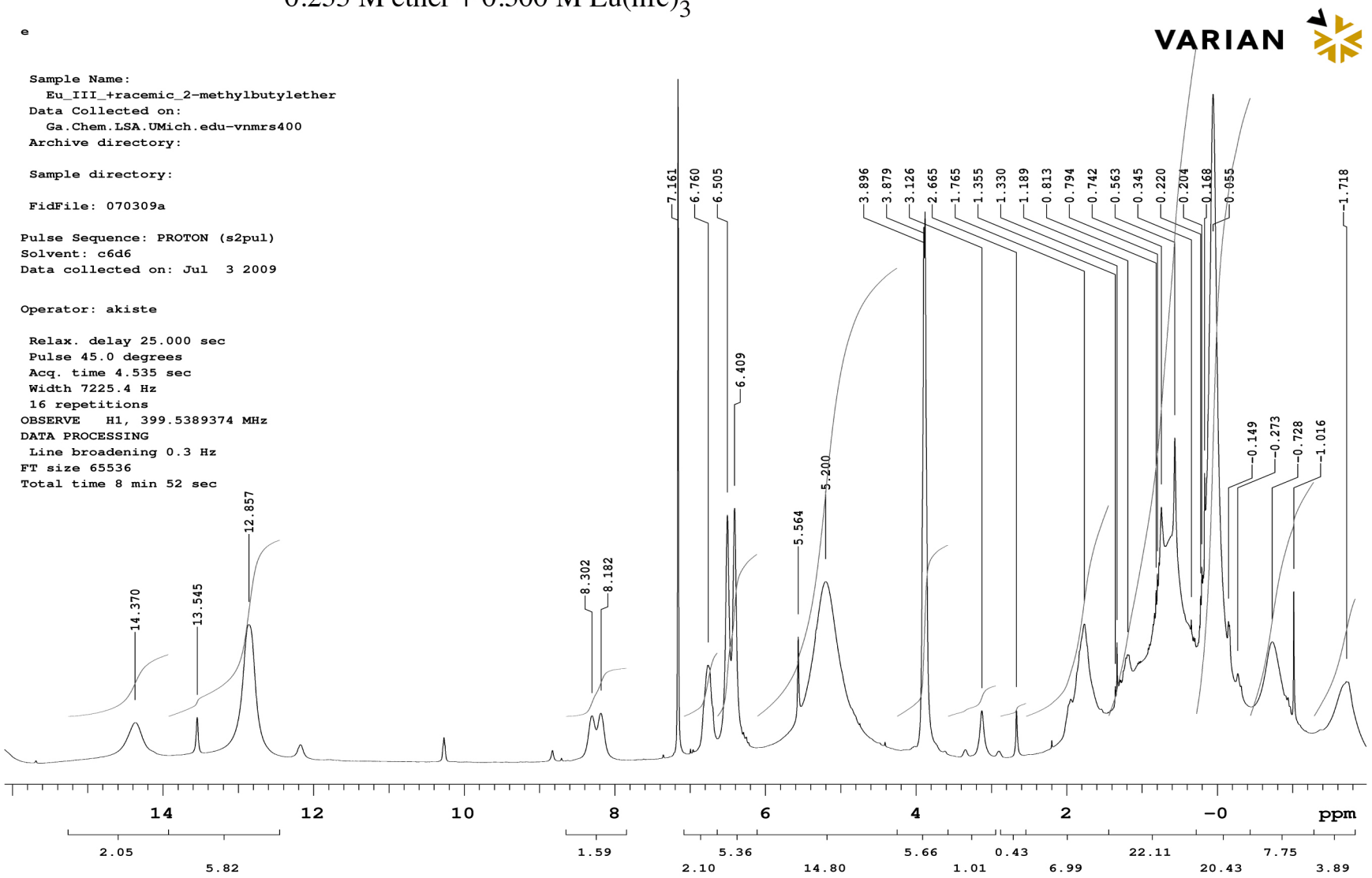
0.235 M ether + 0.142 M $Eu(hfc)_3$



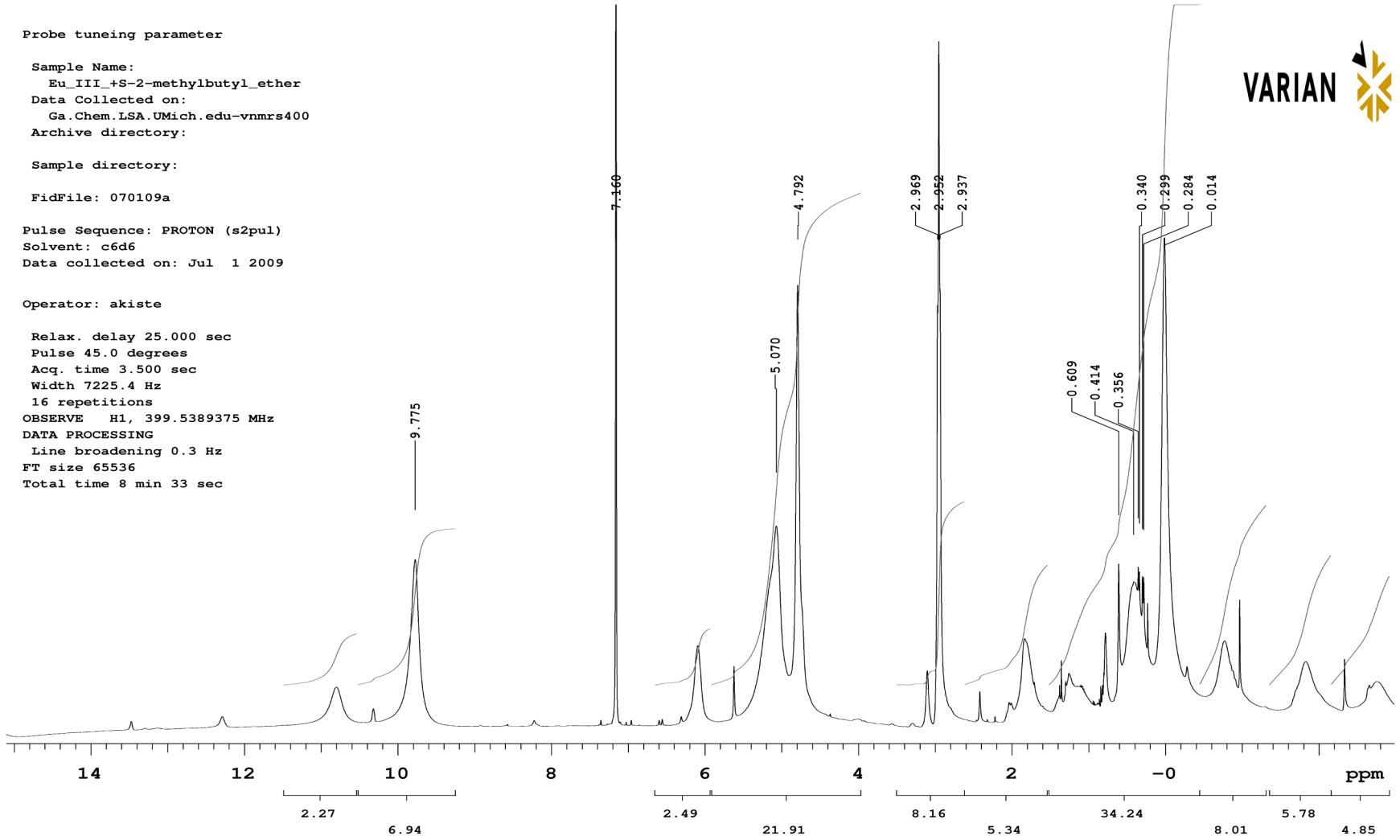
0.235 M ether + 0.202 M $Eu(hfc)_3$



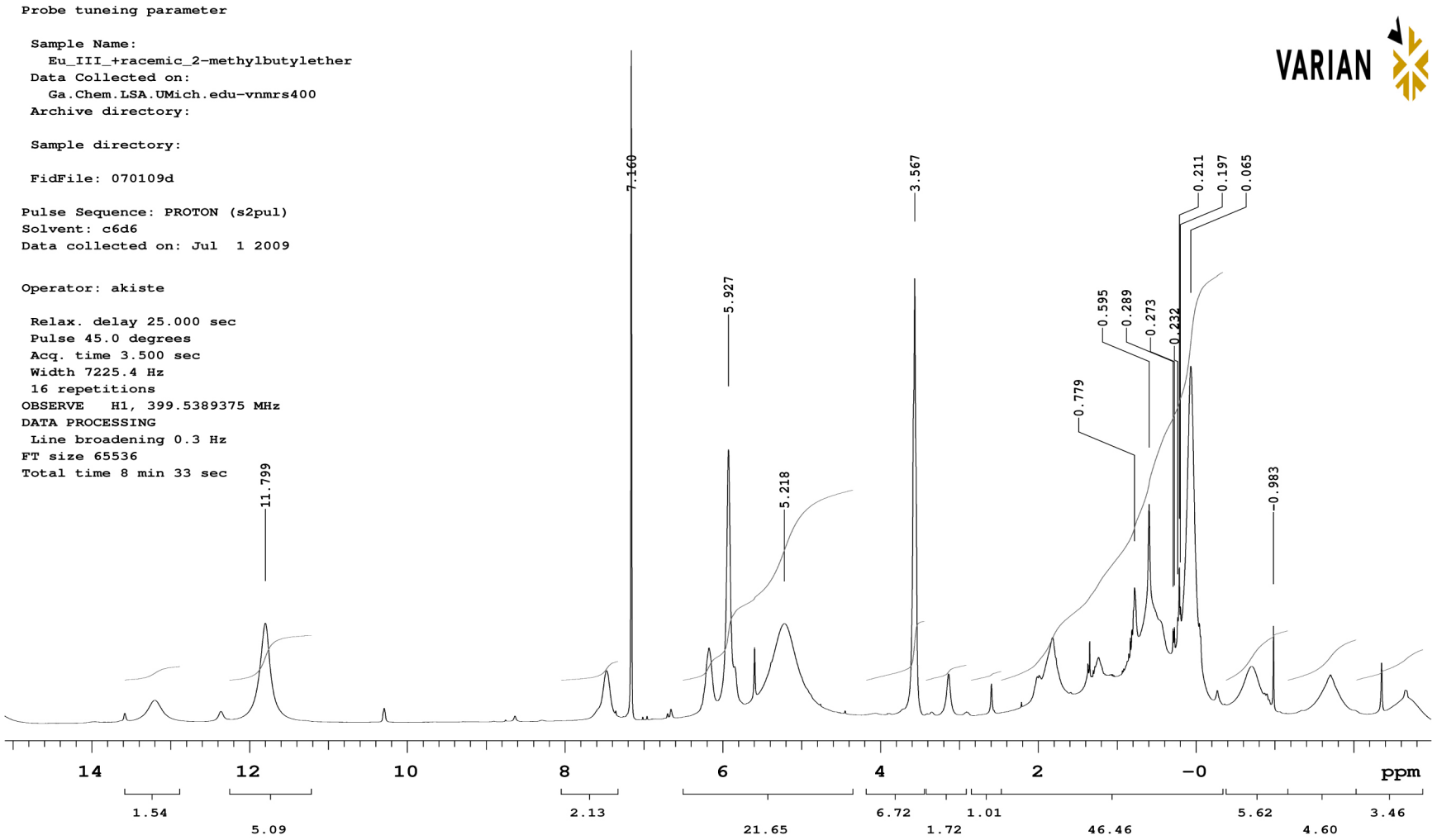
0.235 M ether + 0.300 M $Eu(hfc)_3$



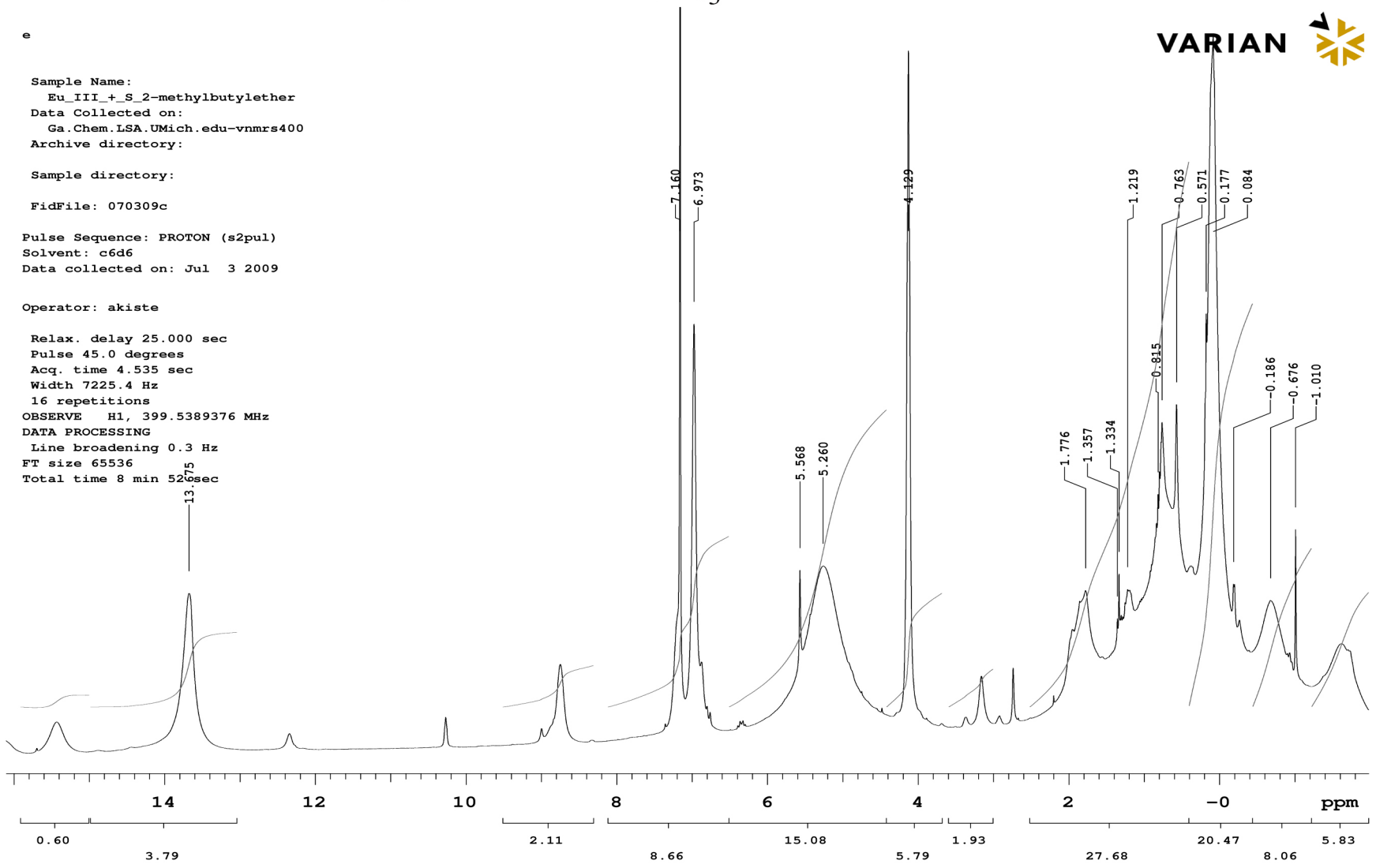
0.183 M (S) ether + 0.152 M $Eu(hfc)_3$



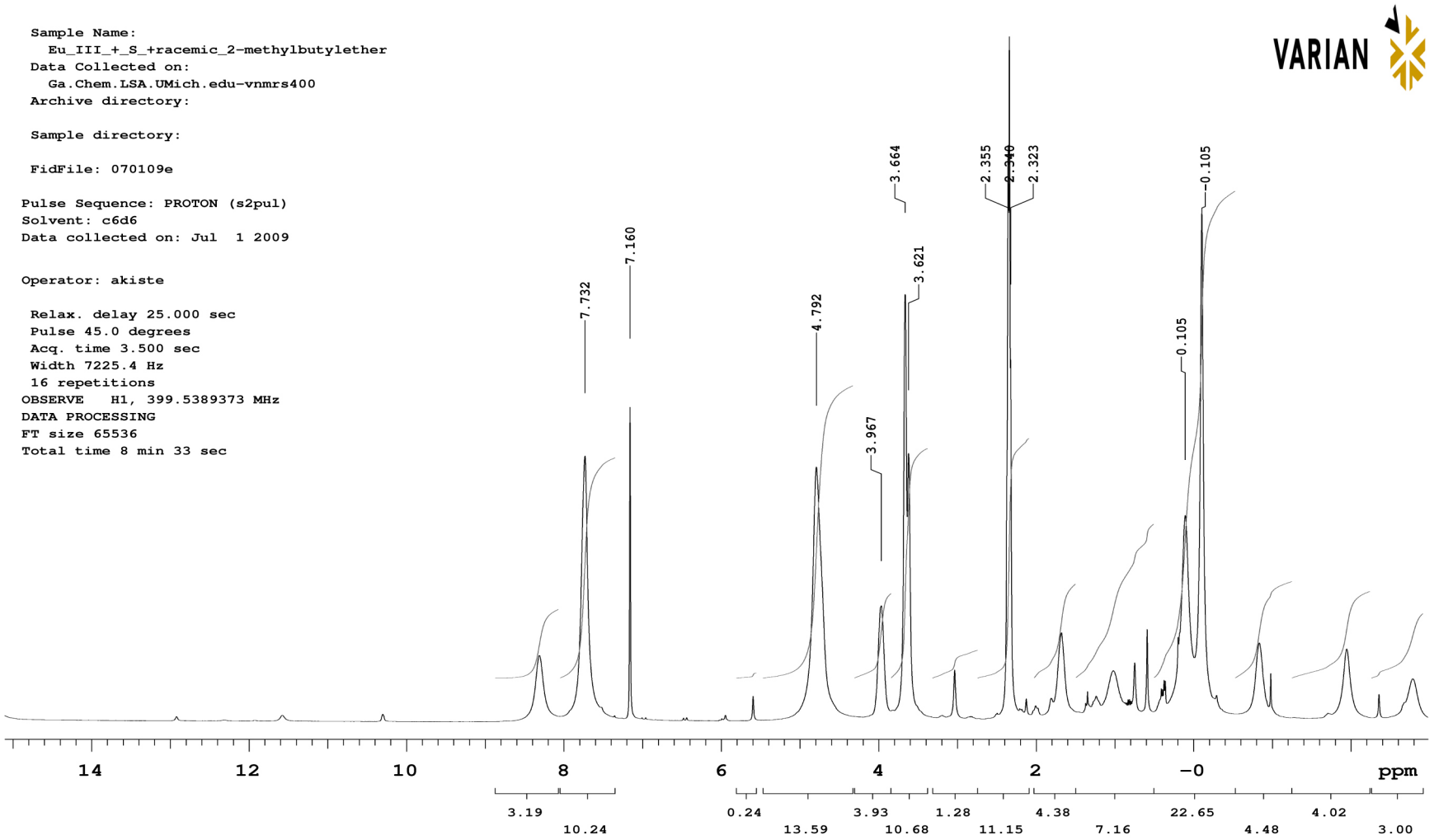
0.183 M (S) ether + 0.212 M $Eu(hfc)_3$



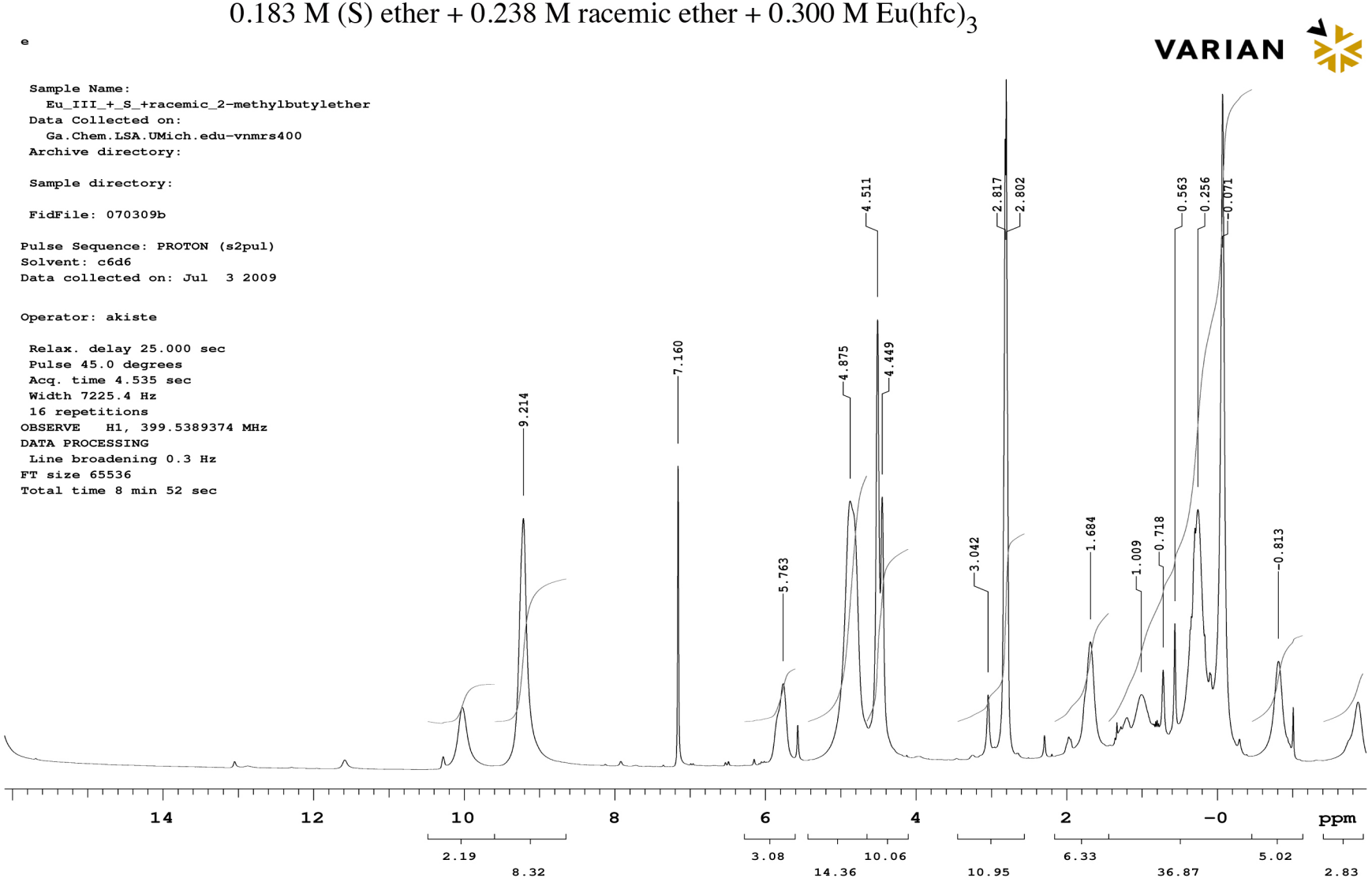
0.183 M (S) ether + 0.300 M $Eu(hfc)_3$

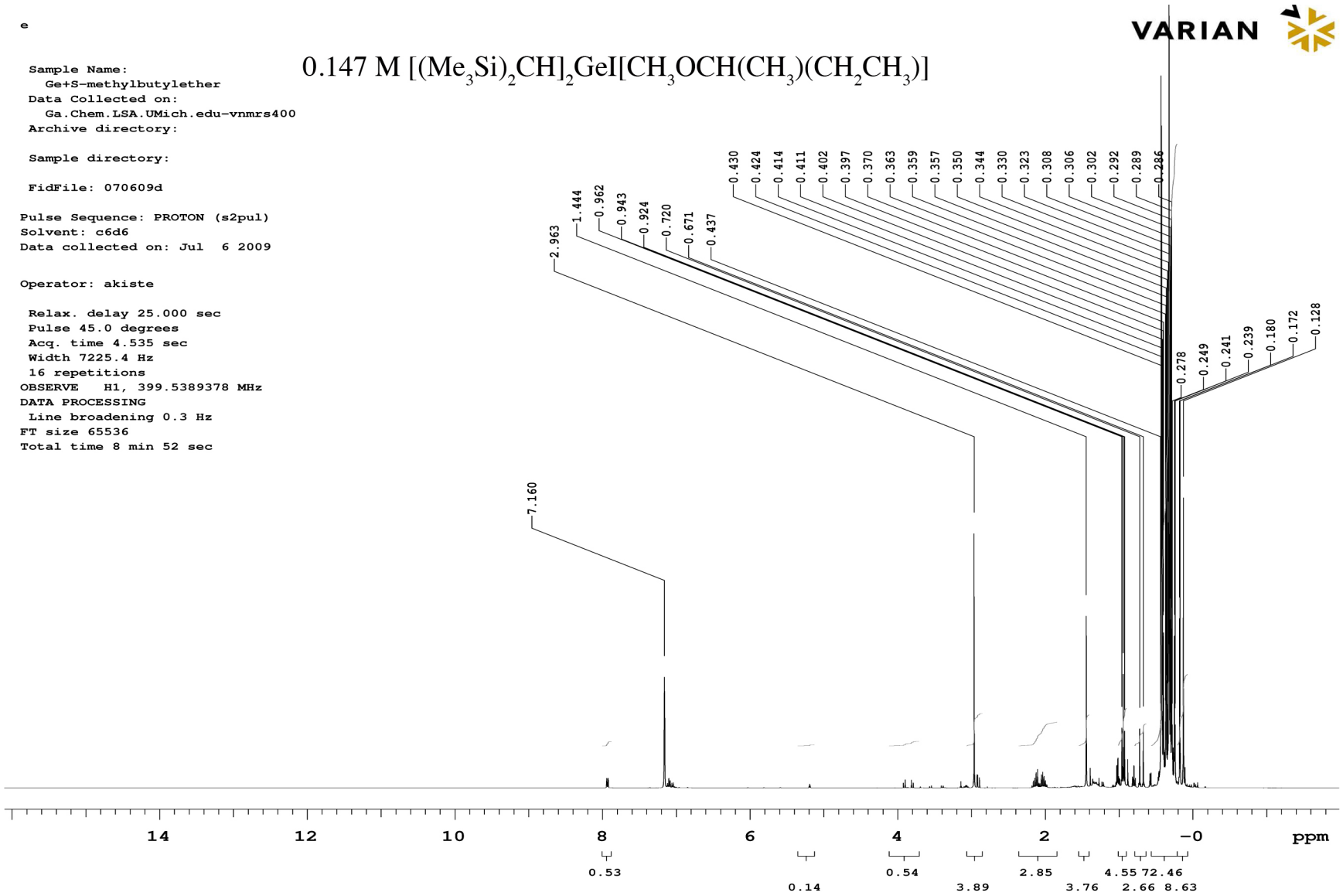


0.183 M (S) ether + 0.238 M racemic ether + 0.152 M $Eu(hfc)_3$



0.183 M (S) ether + 0.238 M racemic ether + 0.300 M $Eu(hfc)_3$



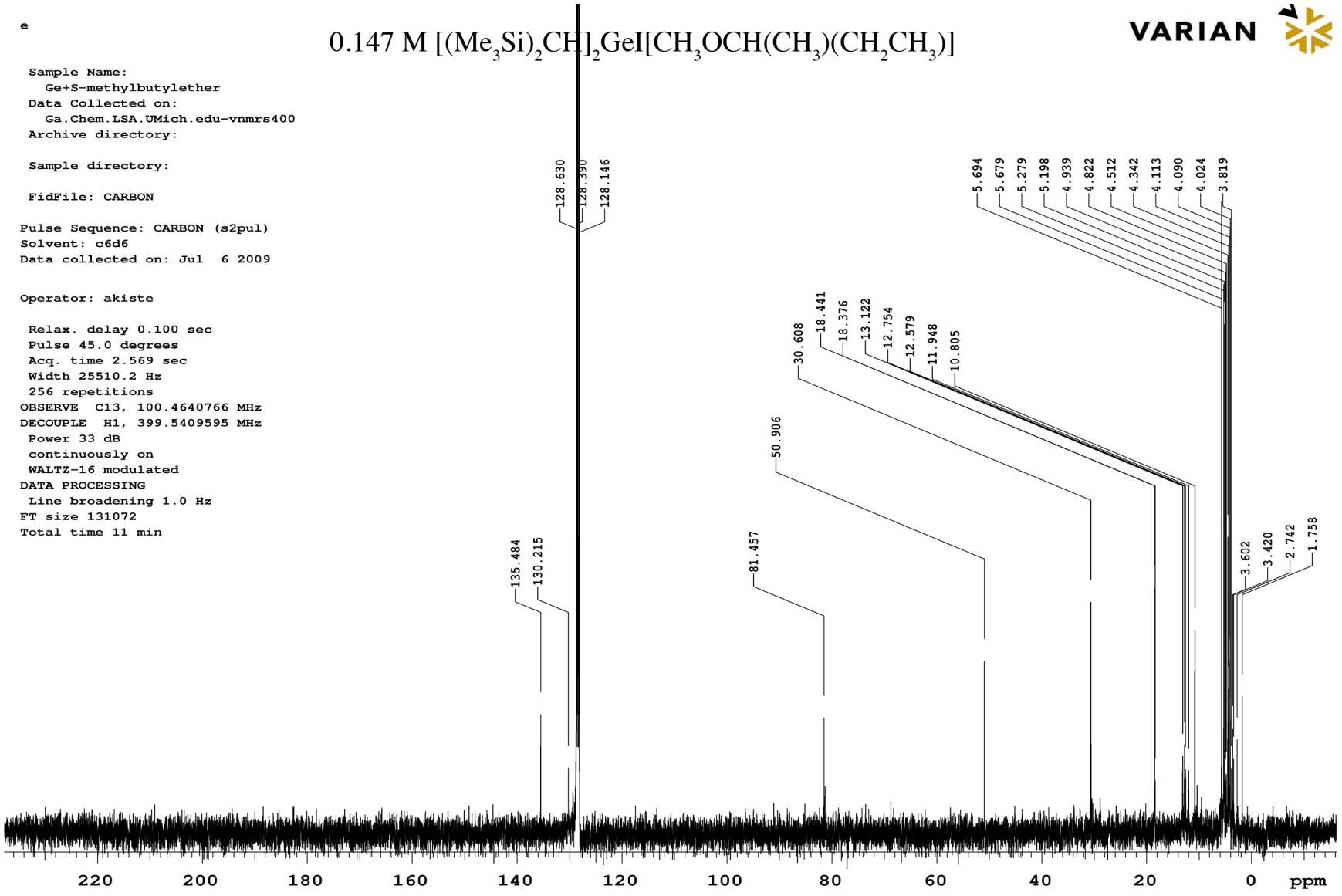

e
Sample Name:
Ge+S-methylbutylether
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070609d
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 6 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389378 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
0.147 M [(Me3Si)2CH]2GeI[CH3OCH(CH3)(CH2CH3)]
VARIAN
7.160
2.963
1.444
0.962
0.943
0.924
0.720
0.671
0.437
0.430
0.424
0.414
0.411
0.402
0.397
0.370
0.363
0.359
0.357
0.350
0.344
0.330
0.323
0.308
0.306
0.302
0.292
0.289
0.286
0.278
0.249
0.241
0.239
0.180
0.172
0.128
14
12
10
8
6
4
2
−0
ppm
0.53
0.14
0.54
3.89
2.85
3.76
4.55
2.66
72.46
8.63

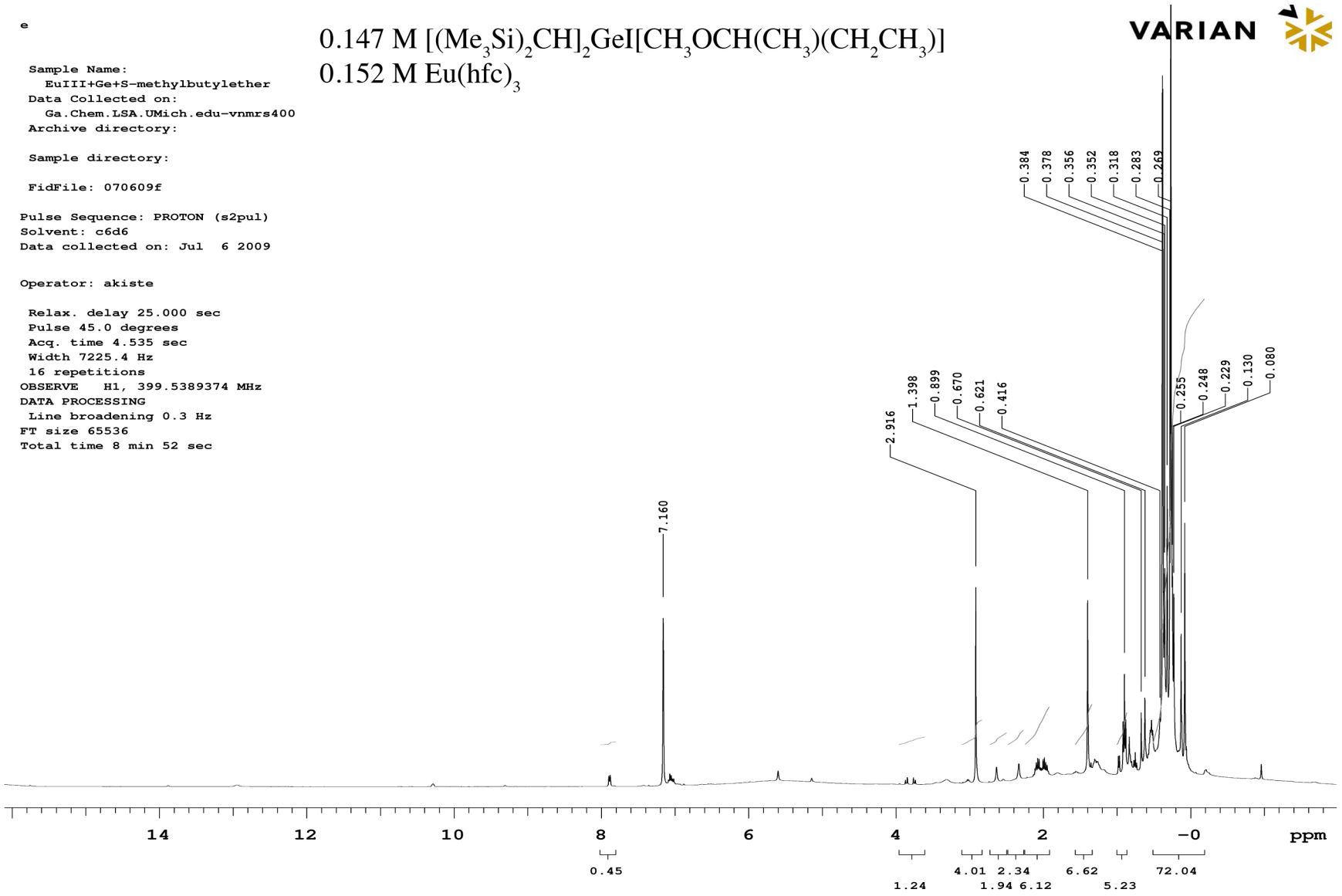
e

0.147 M $[(Me_3Si)_2CH]_2GeI[CH_3OCH(CH_3)(CH_2CH_3)]$

VARIAN

```
 Sample Name:
   Ge+S-methylbutylether
 Data Collected on:
   Ga.Chem.LSA.UMich.edu-vnmrs400
 Archive directory:

 Sample directory:

 FidFile: CARBON

Pulse Sequence: CARBON (s2pul)
Solvent: c6d6
Data collected on: Jul  6 2009

Operator: akiste

 Relax. delay 0.100 sec
 Pulse 45.0 degrees
 Acq. time 2.569 sec
 Width 25510.2 Hz
 256 repetitions
OBSERVE  C13, 100.4640766 MHz
DECOUPLE  H1, 399.5409595 MHz
 Power 33 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.0 Hz
FT size 131072
Total time 11 min
```



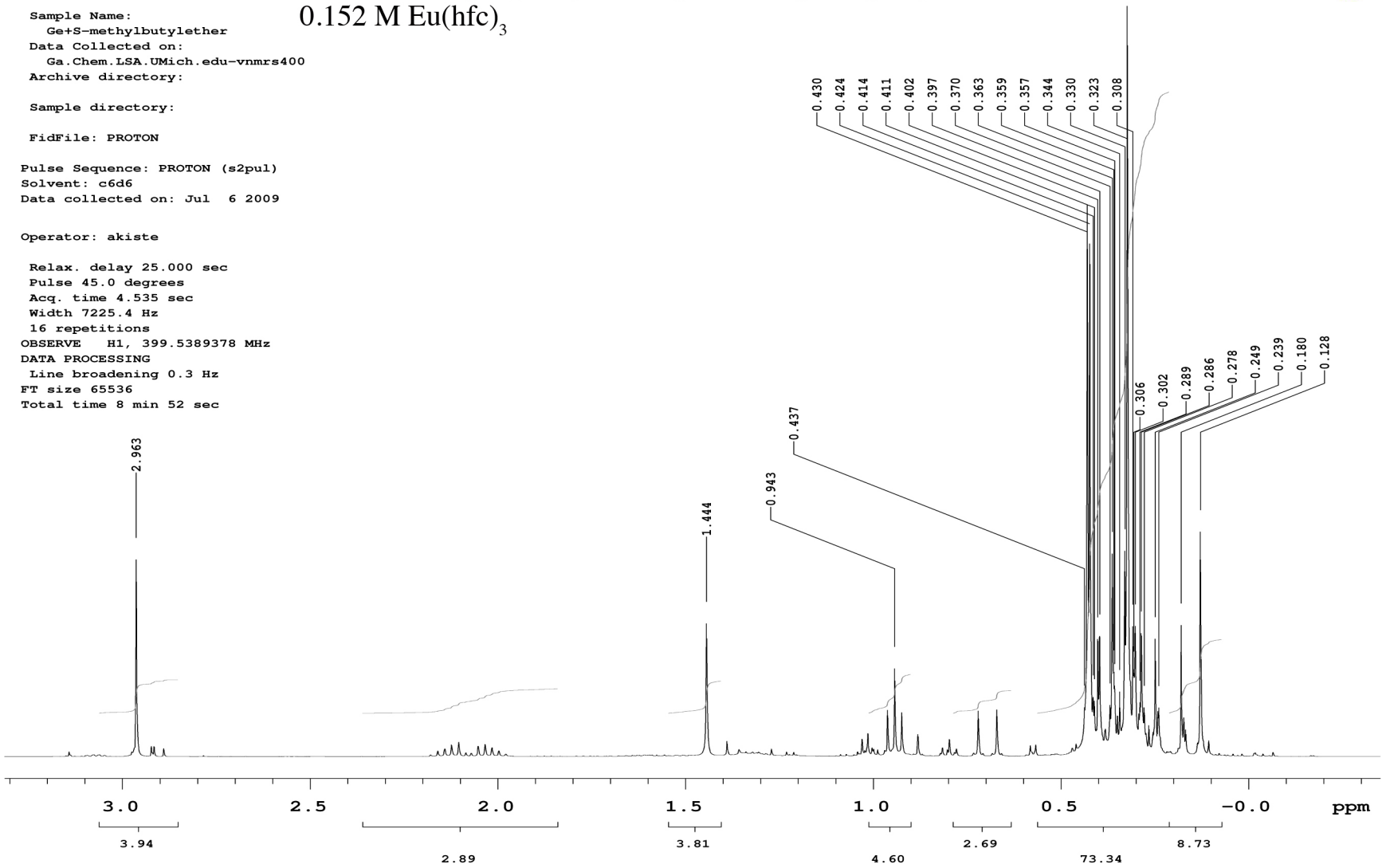

e
Sample Name:
EuIII+Ge+S-methylbutylether
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070609f
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 6 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389374 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
0.147 M [(Me3Si)2CH]2GeI[CH3OCH(CH3)(CH2CH3)]
0.152 M Eu(hfc)3
VARIAN
0.384
0.378
0.356
0.352
0.318
0.283
0.269
2.916
1.398
0.899
0.670
0.621
0.416
0.255
0.248
0.229
0.130
0.080
7.160
14
12
10
8
6
4
2
−0
ppm
0.45
1.24
4.01
1.94
2.34
6.12
6.62
5.23
72.04

e

0.147 M $[(Me_3Si)_2CH]_2GeI[CH_3OCH(CH_3)(CH_2CH_3)]$
0.152 M $Eu(hfc)_3$

VARIAN

```
 Sample Name:
   Ge+S-methylbutylether
 Data Collected on:
   Ga.Chem.LSA.UMich.edu-vnmrs400
 Archive directory:

 Sample directory:

 FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul  6 2009

Operator: akiste

 Relax. delay 25.000 sec
 Pulse 45.0 degrees
 Acq. time 4.535 sec
 Width 7225.4 Hz
 16 repetitions
OBSERVE    H1, 399.5389378 MHz
DATA PROCESSING
 Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
```

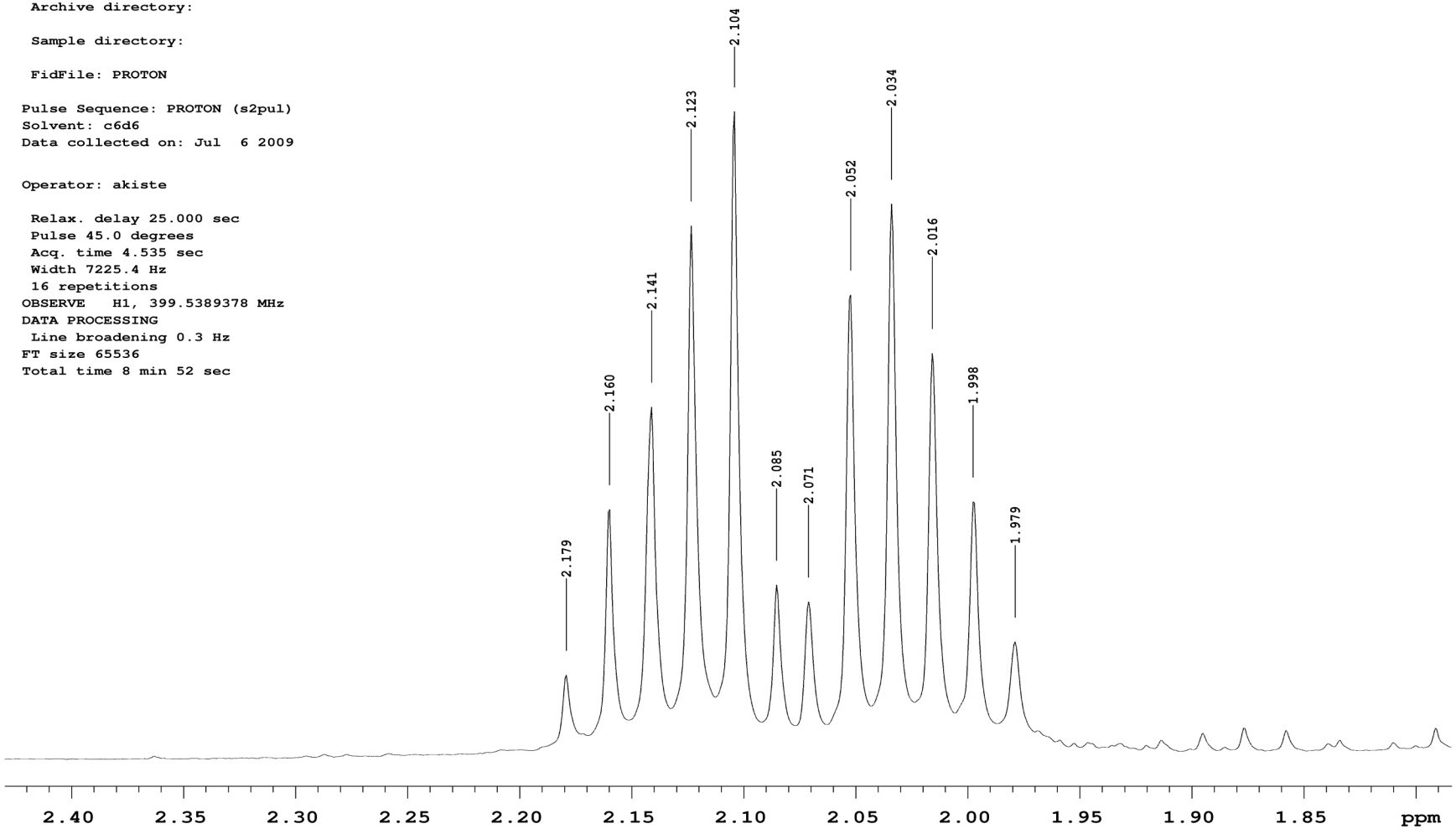


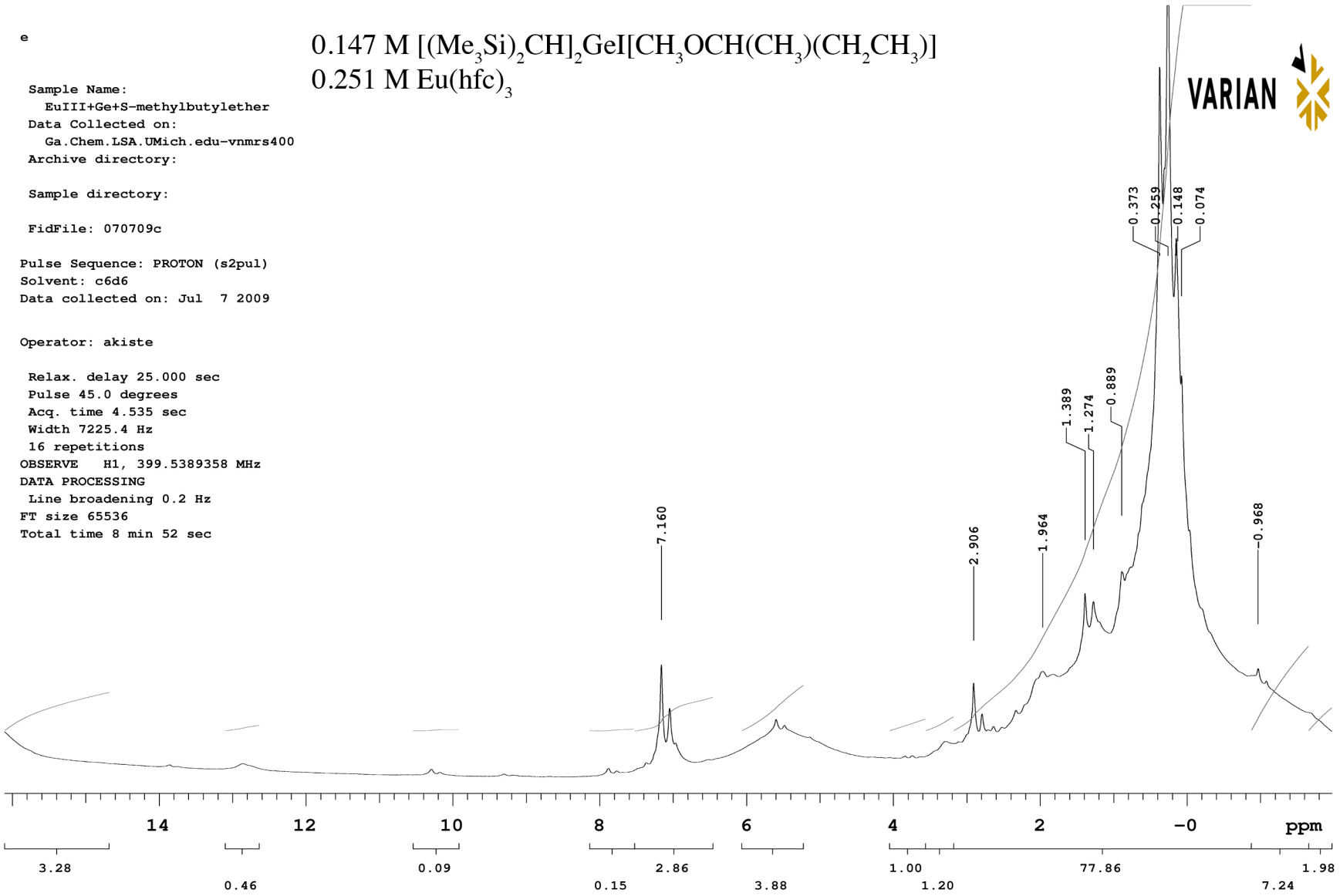
e

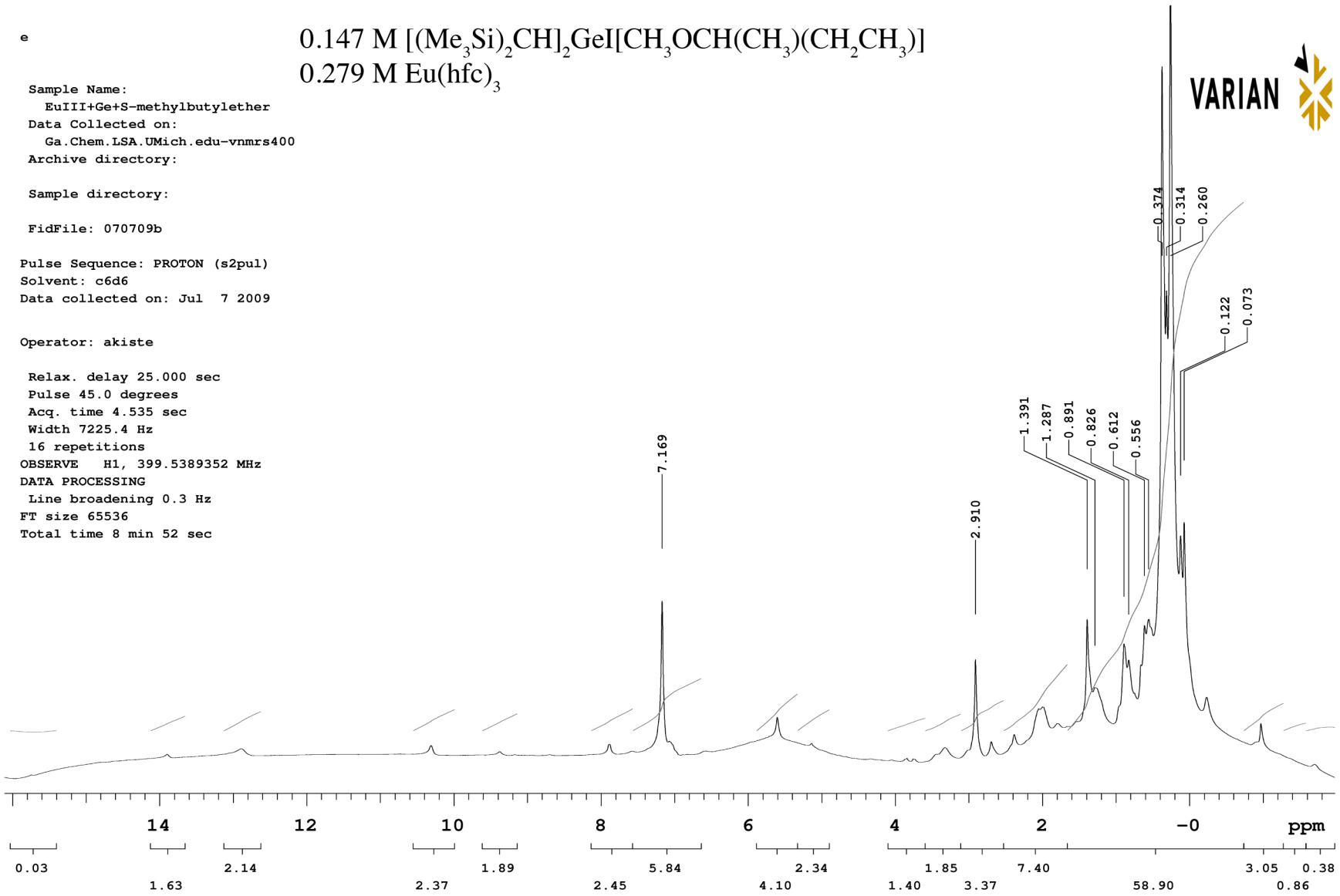
0.147 M $[(Me_3Si)_2CH]_2GeI[CH_3OCH(CH_3)(CH_2CH_3)]$
0.152 M $Eu(hfc)_3$

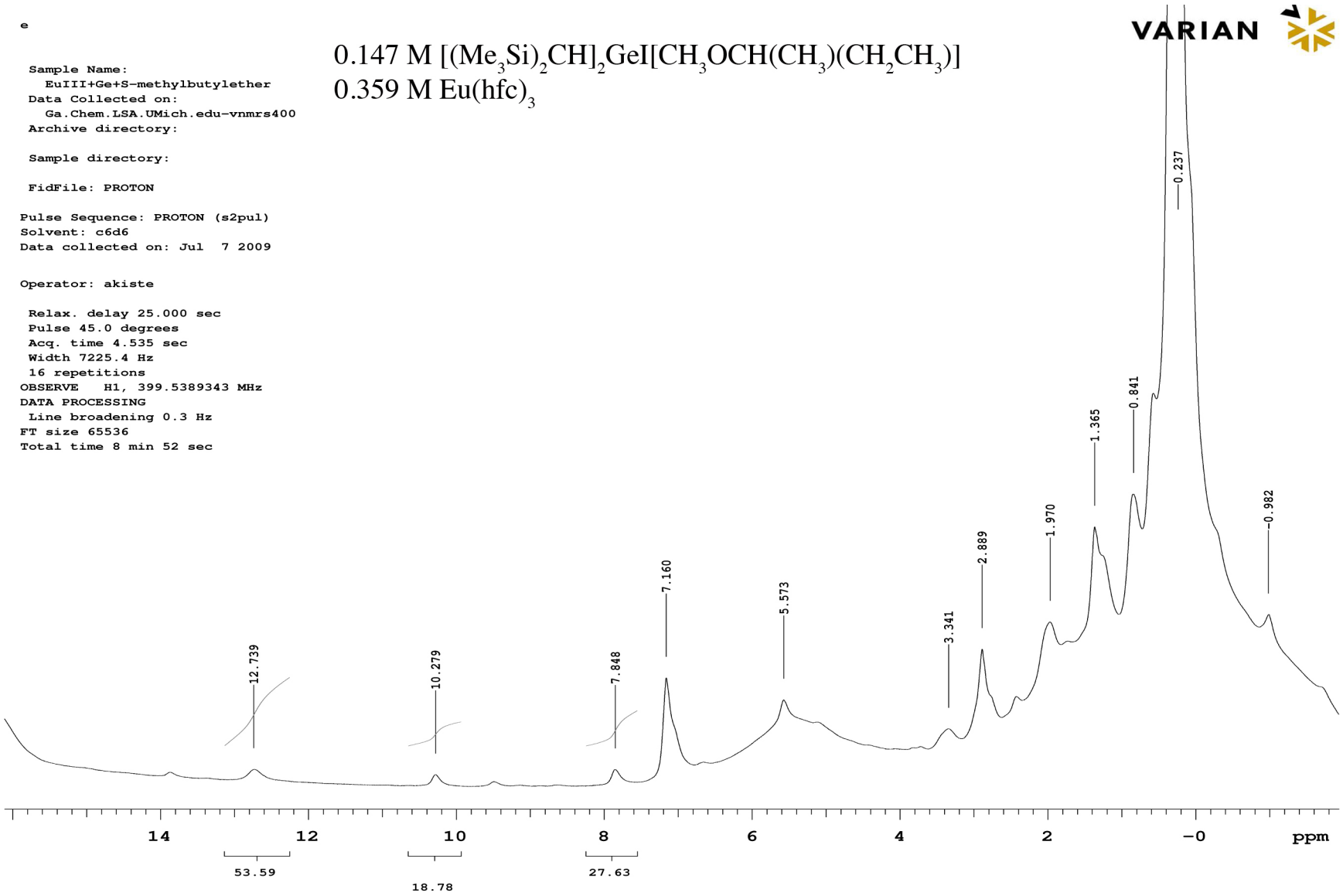
VARIAN

```
 Sample Name:
   Ge+S-methylbutylether
 Data Collected on:
   Ga.Chem.LSA.UMich.edu-vnmrs400
 Archive directory:

 Sample directory:

 FidFile: PROTON

Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul  6 2009

Operator: akiste

 Relax. delay 25.000 sec
 Pulse 45.0 degrees
 Acq. time 4.535 sec
 Width 7225.4 Hz
 16 repetitions
OBSERVE   H1, 399.5389378 MHz
DATA PROCESSING
 Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
```

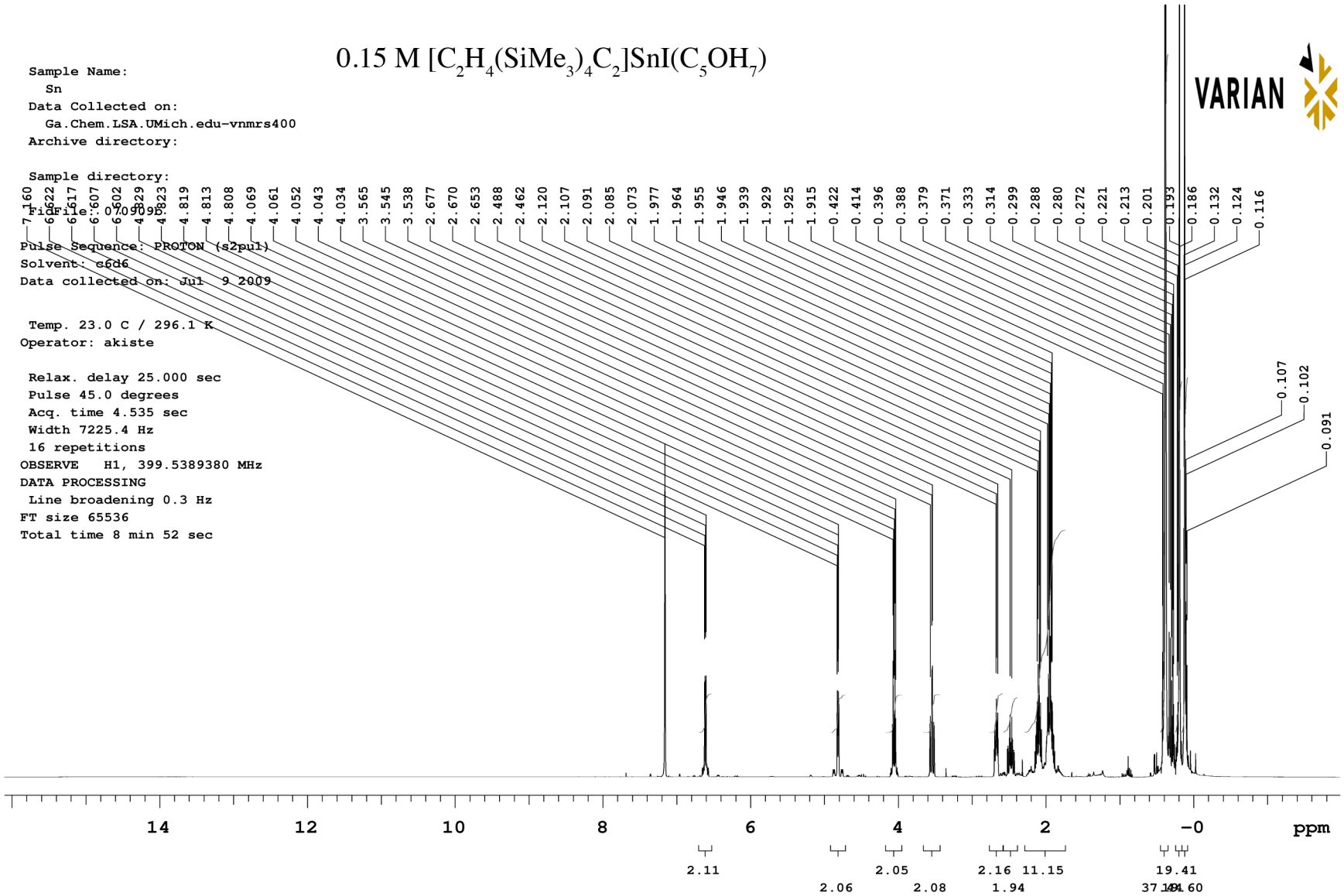



e
0.147 M [(Me3Si)2CH]2GeI[CH3OCH(CH3)(CH2CH3)]
0.251 M Eu(hfc)3
Sample Name:
EuIII+Ge+S-methylbutylether
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070709c
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 7 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389358 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Total time 8 min 52 sec
VARIAN
0.373
0.259
0.148
0.074
1.389
1.274
0.889
7.160
2.906
1.964
0.968
14
12
10
8
6
4
2
−0
ppm
3.28
0.46
0.09
2.86
0.15
3.88
1.00
1.20
77.86
7.24
1.98

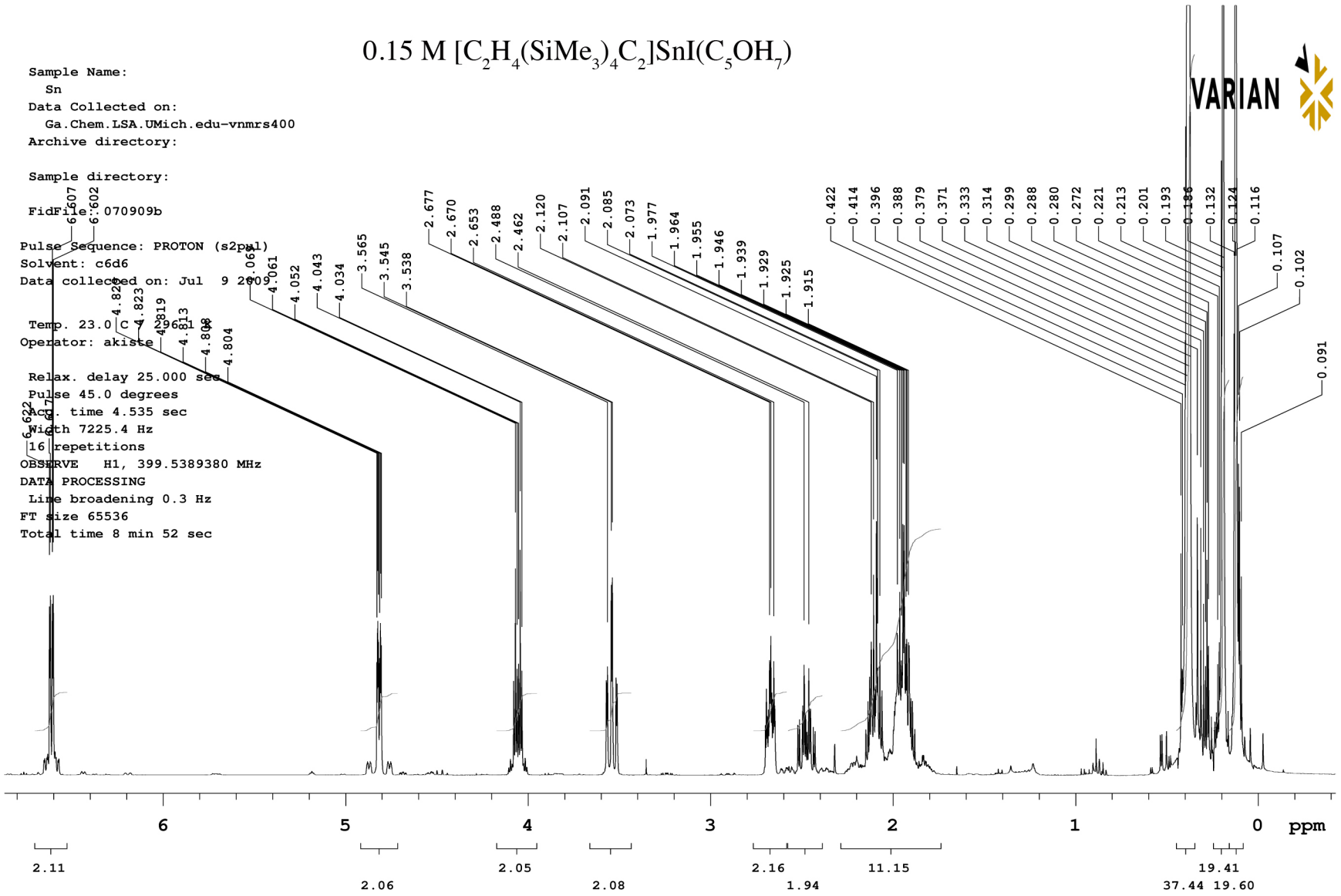

e
0.147 M [(Me3Si)2CH]2GeI[CH3OCH(CH3)(CH2CH3)]
0.279 M Eu(hfc)3
Sample Name:
EuIII+Ge+S-methylbutylether
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070709b
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 7 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389352 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
VARIAN
7.169
2.910
1.391
1.287
0.891
0.826
0.612
0.556
0.374
0.314
0.260
0.122
0.073
14
12
10
8
6
4
2
−0
ppm
0.03
1.63
2.14
2.37
1.89
2.45
5.84
4.10
2.34
1.40
1.85
3.37
7.40
58.90
3.05
0.86
0.38

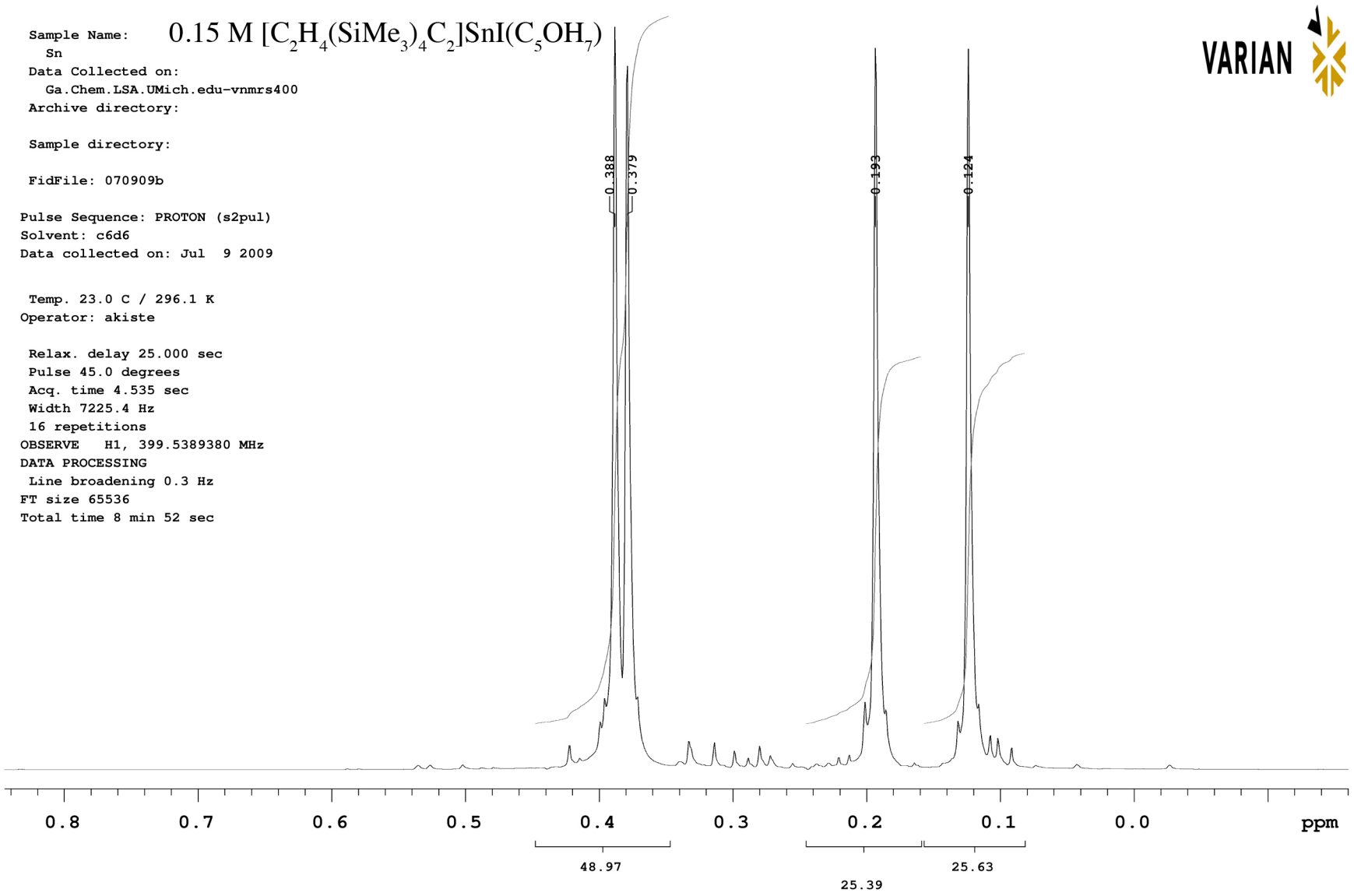

e
Sample Name:
EuIII+Ge+S-methylbutylether
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: PROTON
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 7 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389343 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
0.147 M [(Me3Si)2CH]2GeI[CH3OCH(CH3)(CH2CH3)]
0.359 M Eu(hfc)3
VARIAN
12.739
10.279
7.848
7.160
5.573
3.341
2.889
1.970
1.365
0.841
0.237
-0.982
14
12
10
8
6
4
2
-0
ppm
53.59
18.78
27.63

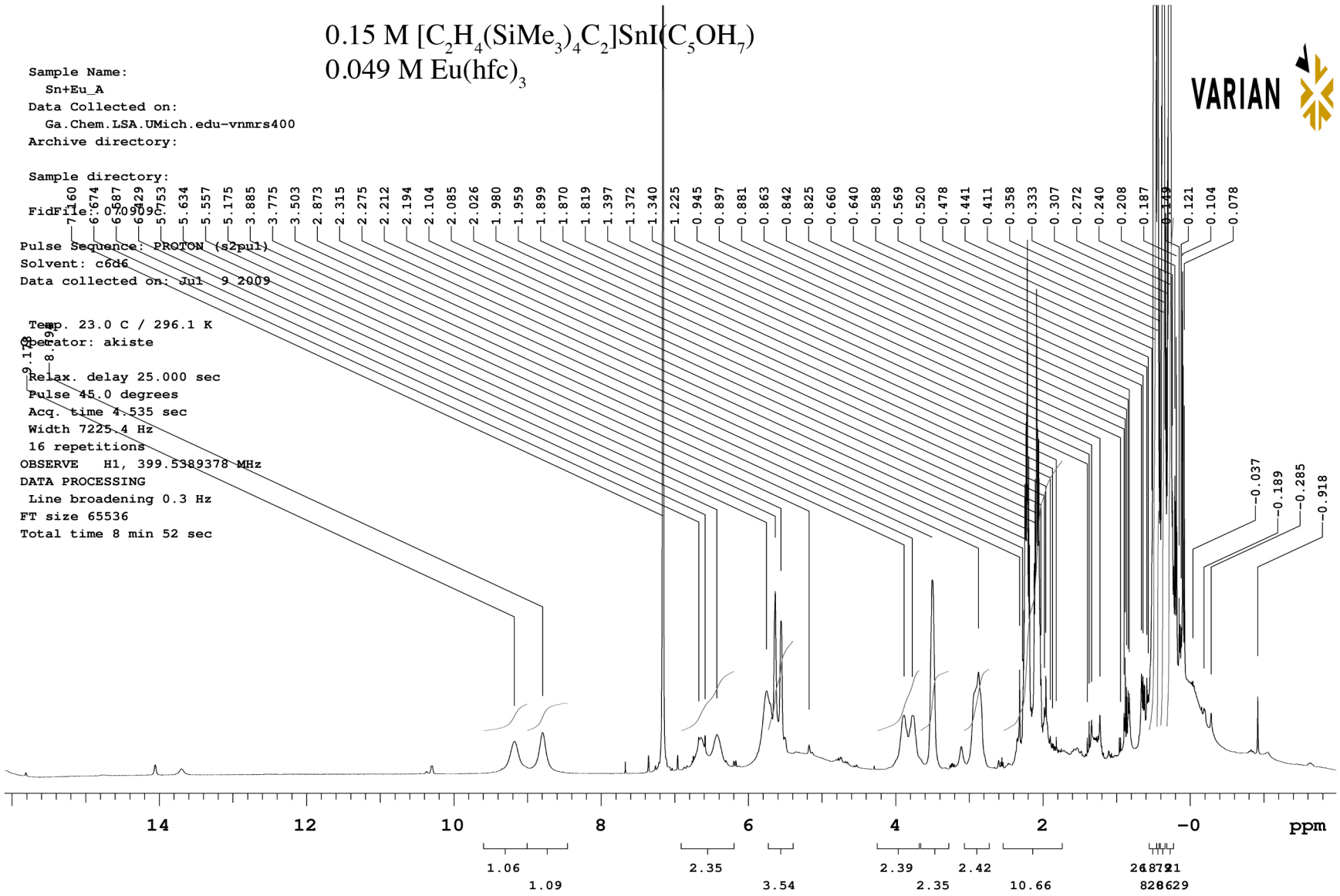
0.15 M $[C_2H_4(SiMe_3)_4C_2]SnI(C_5OH_7)$

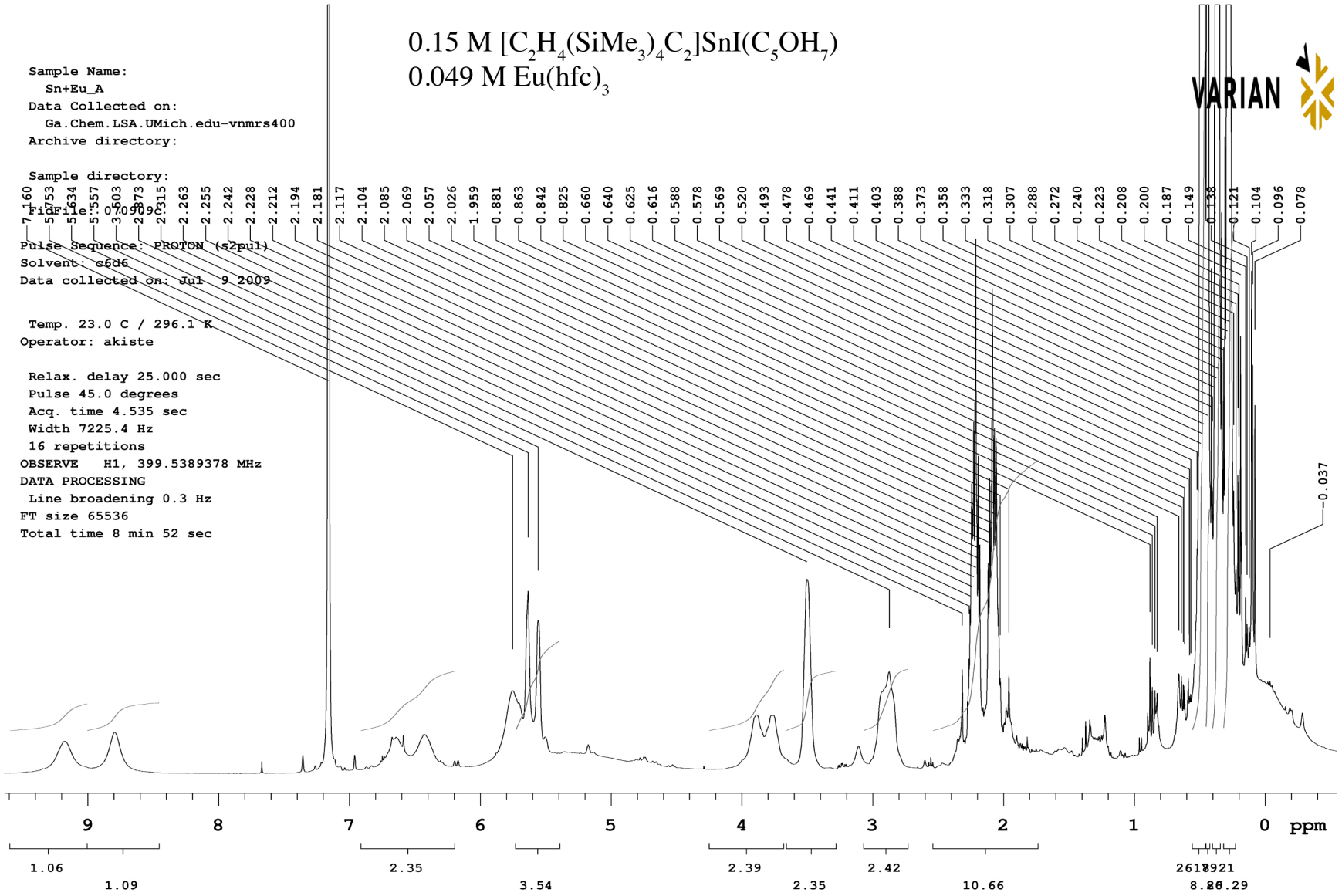


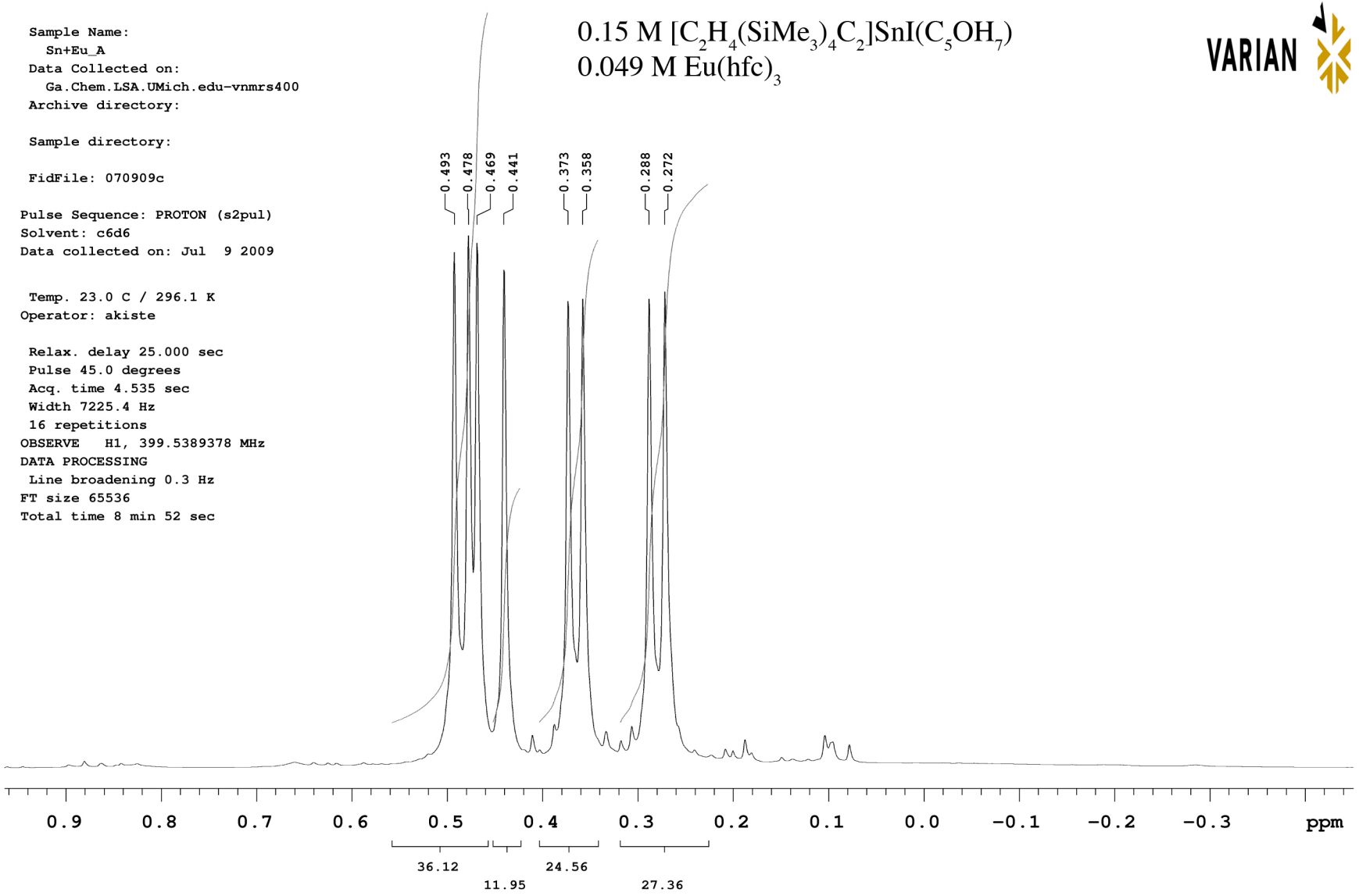
0.15 M $[C_2H_4(SiMe_3)_4C_2]SnI(C_5OH_7)$

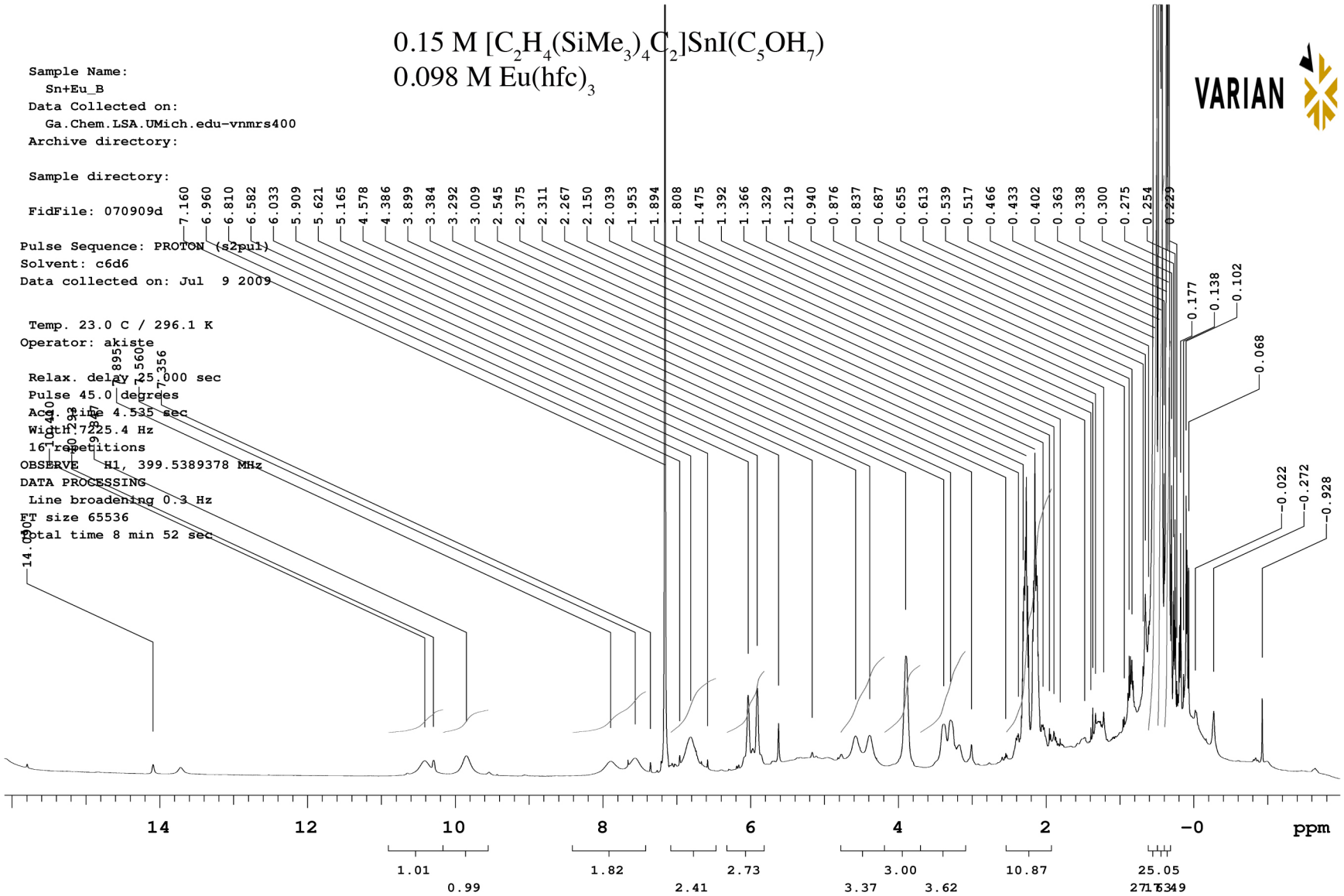


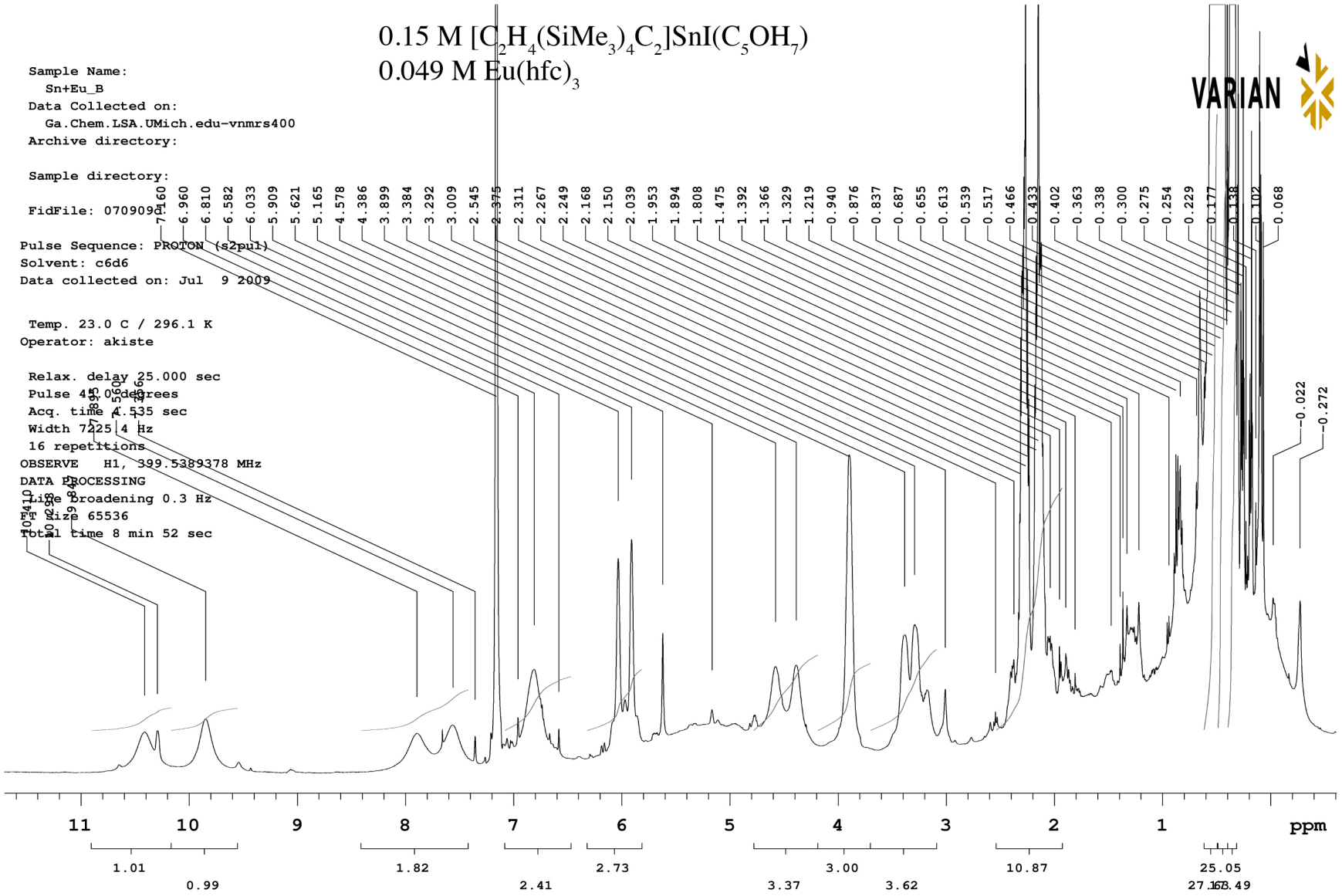

Sample Name:
0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
Sn
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909b
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Temp. 23.0 C / 296.1 K
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389380 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
VARIAN
0.388
0.379
0.193
0.124
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
ppm
48.97
25.39
25.63

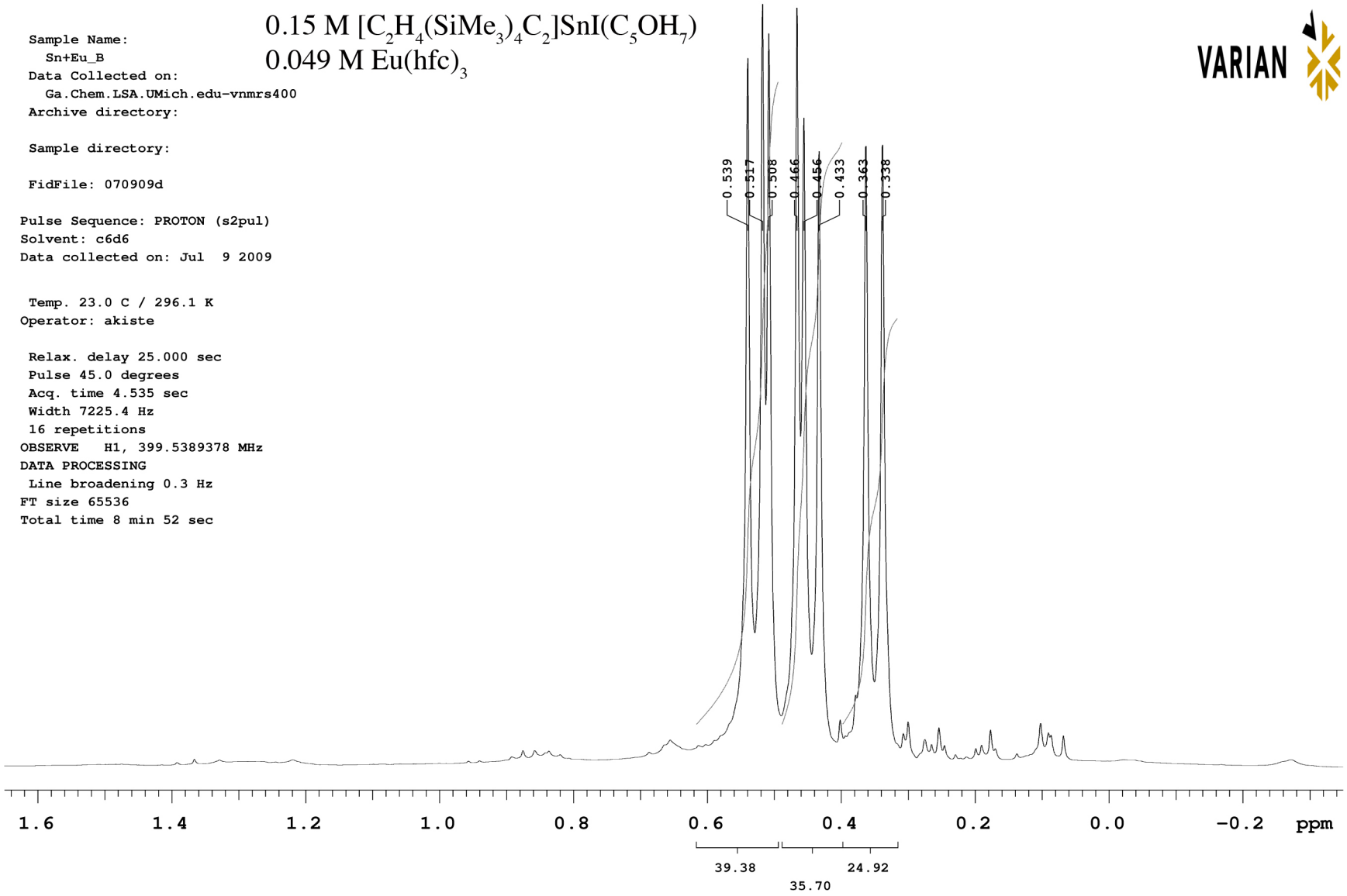

0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.049 M Eu(hfc)3
Sample Name:
Sn+Eu_A
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Temp. 23.0 C / 296.1 K
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389378 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
VARIAN
ppm
1.06
1.09
2.35
3.54
2.39
2.35
2.42
10.66

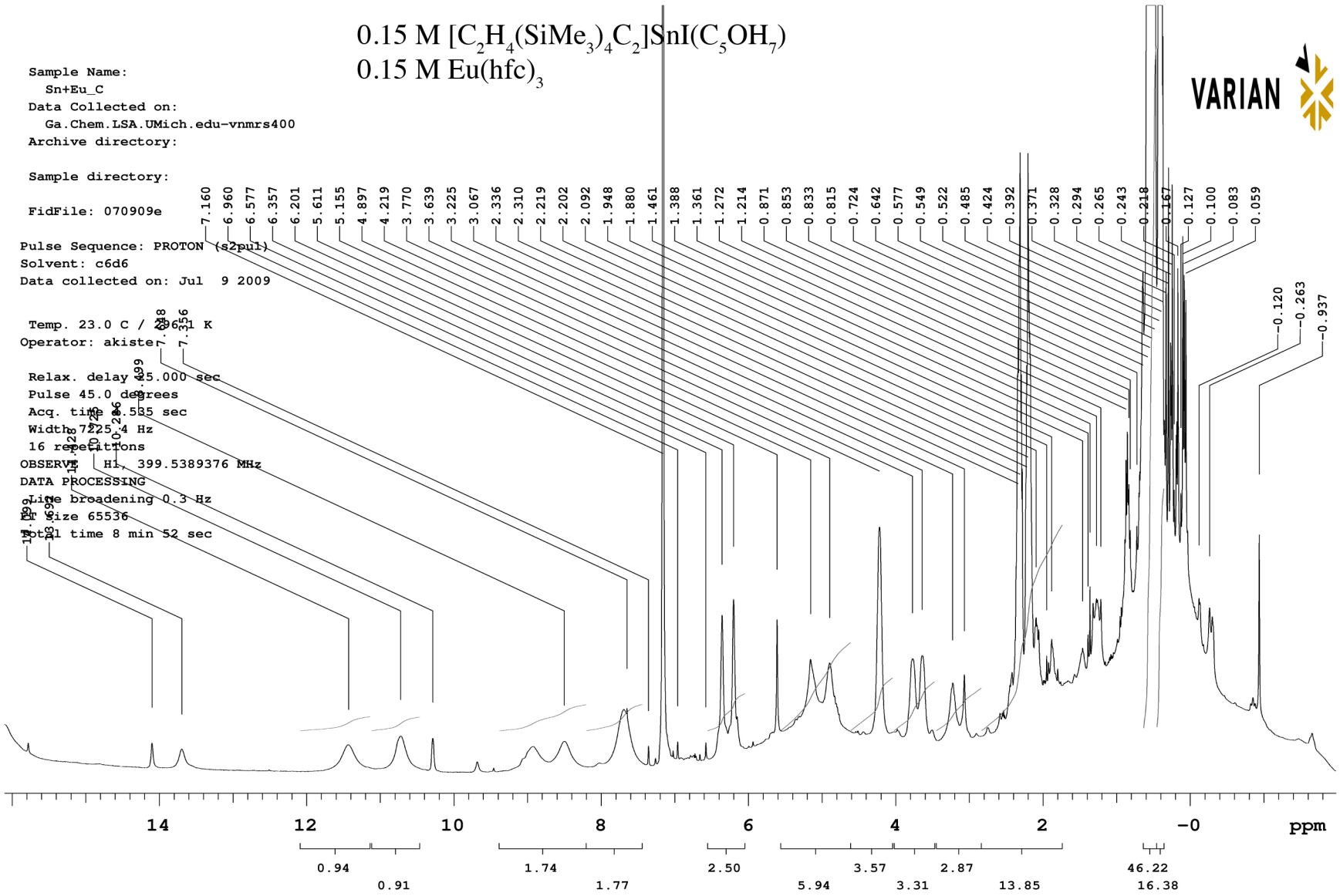

0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.049 M Eu(hfc)3
Sample Name:
Sn+Eu_A
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Temp. 23.0 C / 296.1 K
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389378 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
VARIAN
7.160 5.753 5.634 5.557 5.603 2.873 2.315 2.263 2.255 2.242 2.228 2.212 2.194 2.181 2.117 2.104 2.085 2.069 2.057 2.026 1.959 0.881 0.863 0.842 0.825 0.660 0.640 0.625 0.616 0.588 0.578 0.569 0.520 0.493 0.478 0.469 0.441 0.411 0.403 0.388 0.373 0.358 0.333 0.318 0.307 0.288 0.272 0.240 0.223 0.208 0.200 0.187 0.149 0.138 0.121 0.104 0.096 0.078
-0.037
9 8 7 6 5 4 3 2 1 0 ppm
1.06 1.09 2.35 3.54 2.39 2.35 2.42 10.66 2613 3921 8.26 0.29

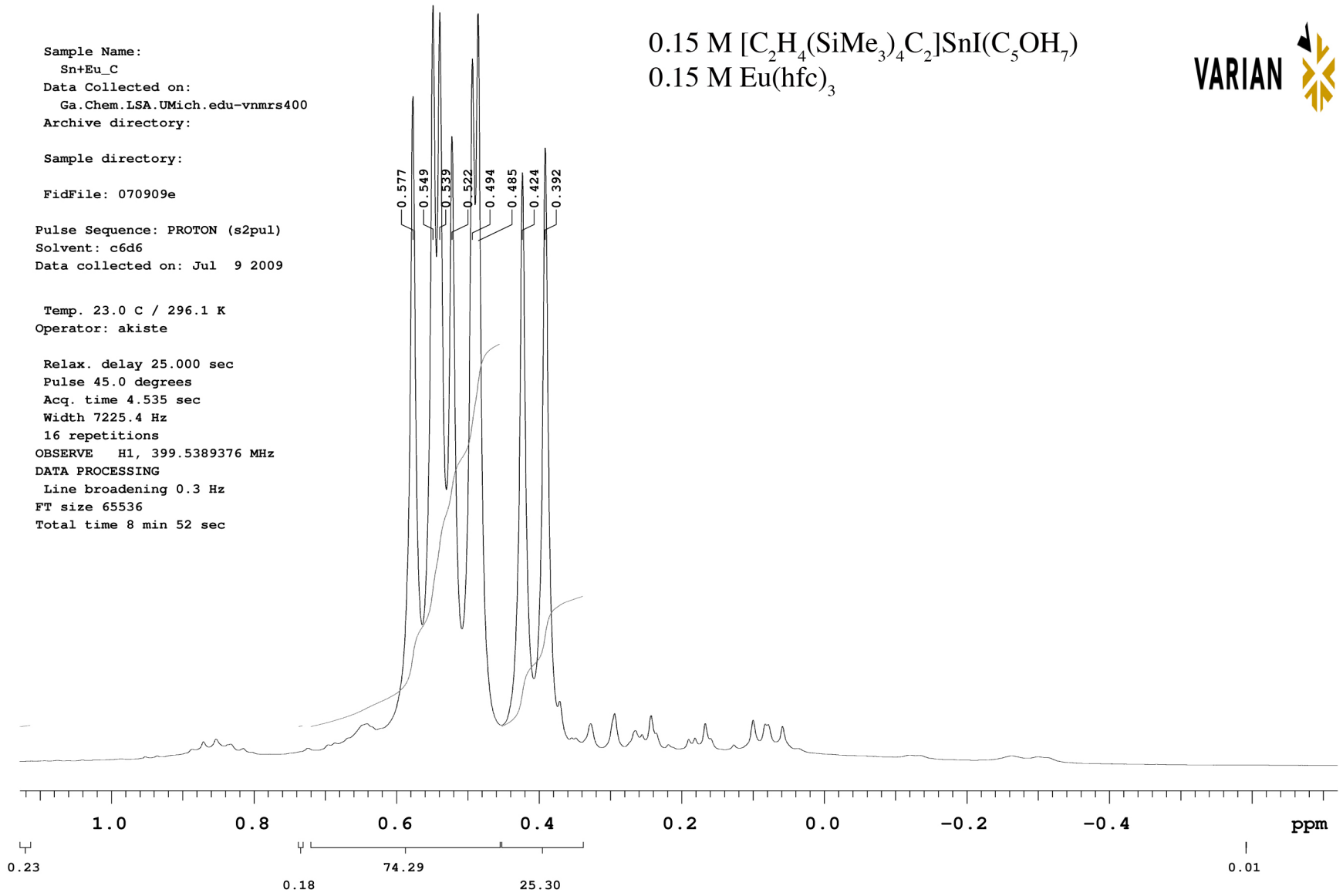

Sample Name:
Sn+Eu_A
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909c
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Temp. 23.0 C / 296.1 K
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389378 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.049 M Eu(hfc)3
VARIAN
0.493
0.478
0.469
0.441
0.373
0.358
0.288
0.272
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
ppm
36.12
11.95
24.56
27.36

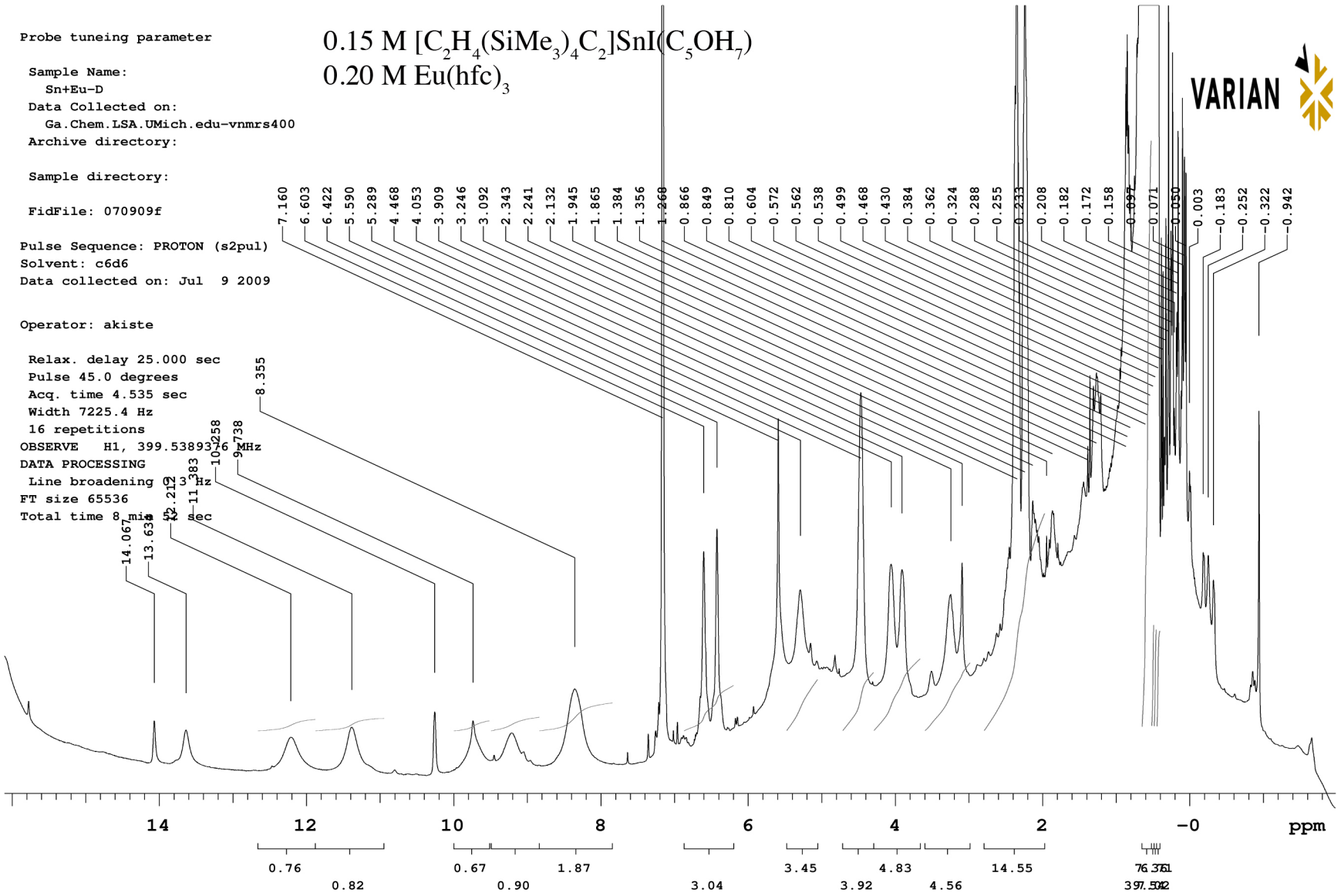

0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.098 M Eu(hfc)3
Sample Name:
Sn+Eu_B
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909d
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Temp. 23.0 C / 296.1 K
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389378 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
7.160
6.960
6.810
6.582
6.033
5.909
5.621
5.165
4.578
4.386
3.899
3.384
3.292
3.009
2.545
2.375
2.311
2.267
2.150
2.039
1.953
1.894
1.808
1.475
1.392
1.366
1.329
1.219
0.940
0.876
0.837
0.687
0.655
0.613
0.539
0.517
0.466
0.433
0.402
0.363
0.338
0.300
0.275
0.254
0.223
0.177
0.138
0.102
0.068
-0.022
-0.272
-0.928
14.090
9.895
9.560
7.356
14
12
10
8
6
4
2
-0
ppm
1.01
0.99
1.82
2.41
2.73
3.00
3.37
3.62
10.87
25.05
27.16
5.49

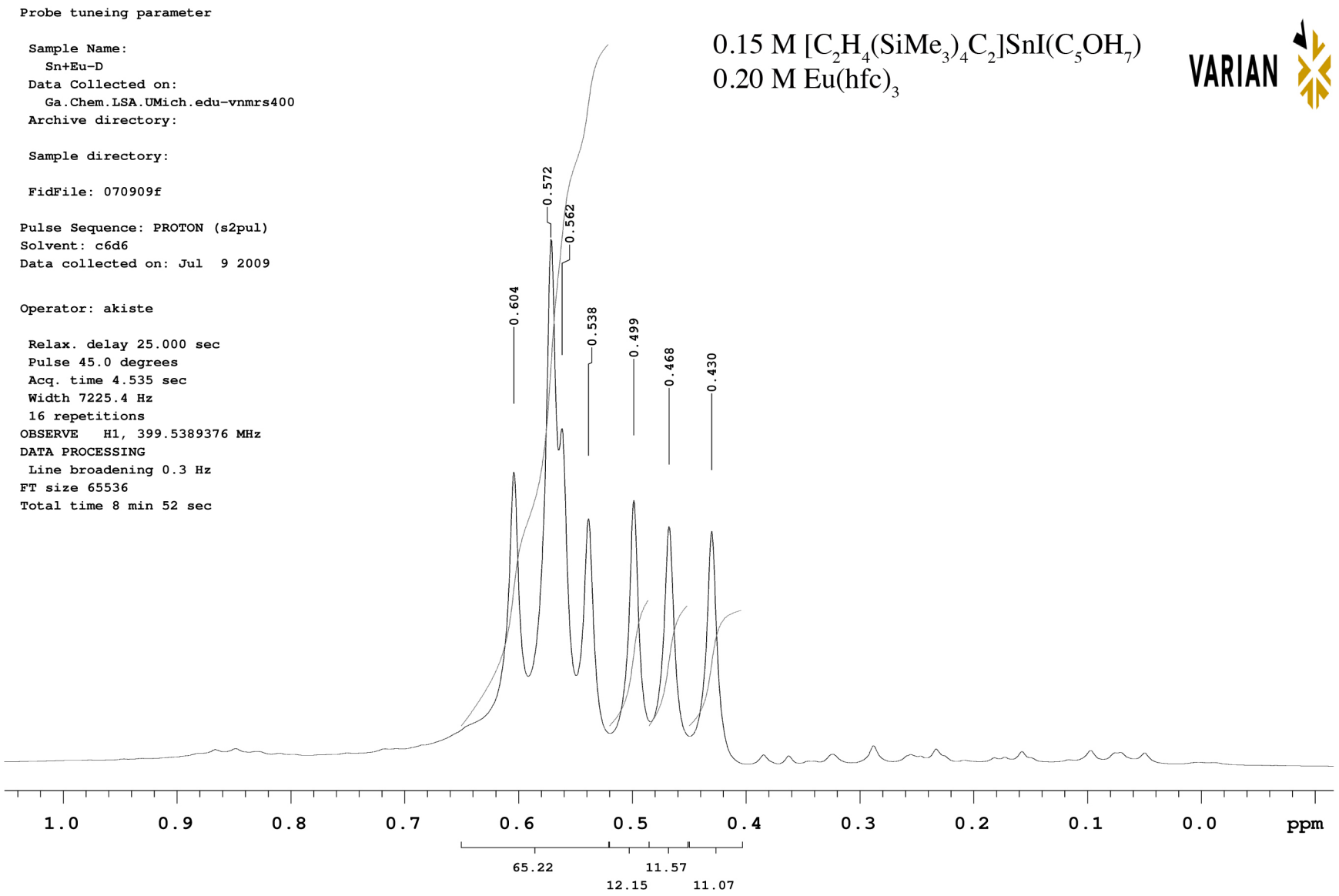

0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.049 M Eu(hfc)3
Sample Name:
Sn+Eu_B
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 0709094
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Temp. 23.0 C / 296.1 K
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389378 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
VARIAN
7.160
6.960
6.810
6.582
6.033
5.909
5.621
5.165
4.578
4.386
3.899
3.384
3.292
3.009
2.545
2.375
2.311
2.267
2.249
2.168
2.150
2.039
1.953
1.894
1.808
1.475
1.392
1.366
1.329
1.219
0.940
0.876
0.837
0.687
0.655
0.613
0.539
0.517
0.466
0.433
0.402
0.363
0.338
0.300
0.275
0.254
0.229
0.177
0.138
0.102
0.068
-0.022
-0.272
11
10
9
8
7
6
5
4
3
2
1
ppm
1.01
0.99
1.82
2.41
2.73
3.00
3.37
3.62
10.87
25.05
27.16
3.49


0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.049 M Eu(hfc)3
Sample Name:
Sn+Eu_B
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909d
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Temp. 23.0 C / 296.1 K
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389378 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
VARIAN
0.539
0.517
0.508
0.466
0.456
0.433
0.363
0.338
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
ppm
39.38
24.92
35.70


0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.15 M Eu(hfc)3
Sample Name:
Sn+Eu_C
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909e
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Temp. 23.0 C / 296.1 K
Operator: akister
Relax. delay 5.000 sec
Pulse 45.0 degrees
Acq. time 3.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389376 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
VARIAN
7.160
6.960
6.577
6.357
6.201
5.611
5.155
4.897
4.219
3.770
3.639
3.225
3.067
2.336
2.310
2.219
2.202
2.092
1.948
1.880
1.461
1.388
1.361
1.272
1.214
0.871
0.853
0.833
0.815
0.724
0.642
0.577
0.549
0.522
0.485
0.424
0.392
0.371
0.328
0.294
0.265
0.243
0.218
0.167
0.127
0.100
0.083
0.059
0.120
0.263
0.937
14
12
10
8
6
4
2
−0
ppm
0.94
0.91
1.74
1.77
2.50
3.57
2.87
5.94
3.31
13.85
46.22
16.38


Sample Name:
Sn+Eu_C
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909e
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Temp. 23.0 C / 296.1 K
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389376 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.15 M Eu(hfc)3
VARIAN
0.577
0.549
0.539
0.522
0.494
0.485
0.424
0.392
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
ppm
0.23
0.18
74.29
25.30
0.01


0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.20 M Eu(hfc)3
VARIAN
Probe tuneing parameter
Sample Name:
Sn+Eu-D
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909f
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389376 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min, 52 sec
7.160
6.603
6.422
5.590
5.289
4.468
4.053
3.909
3.246
3.092
2.343
2.241
2.132
1.945
1.865
1.384
1.356
1.260
0.866
0.849
0.810
0.604
0.572
0.562
0.538
0.499
0.468
0.430
0.384
0.362
0.324
0.288
0.255
0.233
0.208
0.182
0.172
0.158
0.097
0.071
0.050
0.003
-0.183
-0.252
-0.322
-0.942
8.355
10.258
9.738
11.383
12.212
13.634
14.067
14
12
10
8
6
4
2
-0
ppm
0.76
0.82
0.67
0.90
1.87
3.04
3.45
3.92
4.83
4.56
14.55
76.376
397.502


Probe tuneing parameter
Sample Name:
Sn+Eu-D
Data Collected on:
Ga.Chem.LSA.UMich.edu-vnmrs400
Archive directory:
Sample directory:
FidFile: 070909f
Pulse Sequence: PROTON (s2pul)
Solvent: c6d6
Data collected on: Jul 9 2009
Operator: akiste
Relax. delay 25.000 sec
Pulse 45.0 degrees
Acq. time 4.535 sec
Width 7225.4 Hz
16 repetitions
OBSERVE H1, 399.5389376 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 65536
Total time 8 min 52 sec
0.15 M [C2H4(SiMe3)4C2]SnI(C5OH7)
0.20 M Eu(hfc)3
VARIAN
0.604
0.572
0.562
0.538
0.499
0.468
0.430
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
ppm
65.22
11.57
12.15
11.07

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