

Spectroscopy Rubric

| | | Beginning (0) | Developing (2.6) | Adequate (3) | Accomplished (3.4) | Mastery (4) |
|-----------|-------------------------|--|--|--|--|---|
| Mass Spec | Rule 13/13C isotope | Not used | Rule 13 or 13C used, however error resulting in >±2 carbons obtained | Rule 13 or 13C used, however error resulting in ±2 carbons obtained | Rule 13 or 13C used, however error resulting in ±1 carbon obtained | Number of carbons calculated correctly |
| | MW | Not Found | Incorrect number of carbons identified, molecular formula does not match molecular ion mass | Incorrect number of carbons identified, however molecular formula matches molecular ion mass | Correct number of carbons found, and formula matches the molecular ion mass, however molecular formula incorrect for other reasons | Correct Molecular Formula Found |
| | Isotope N,X | Not Found | | | | Significant isotope effects correctly interpreted |
| | Decomposition Products | Not Found | Few decomposition products calculated, no structural significance noted | Few decomposition products calculated, however significant misinterpretations present, leading to significant errors in corresponding substructures | Some decomposition signals correctly identified, however minor misinterpretations present, leading to minor errors in corresponding substructures | Significant decomposition signals correctly identified with corresponding substructure |
| IR | Functional Groups | No determinations made or all determinations incorrect | Some functional groups determined, however significant misinterpretations present, leading to significant errors | Most functional groups determined, however significant misinterpretations present, leading to significant errors | Most functional groups determined, however minor misinterpretations present, leading to minor errors | All significant functional groups correctly identified. Functional groups not present identified as such. |
| HNMR | # Chemical Environ. | No determination made | Number of chemical environments incorrectly identified, ±2 units | Minor error in determination of chemical environments, ±1 unit | Number of chemical environments determined, however determination is incorrect due to overlapping signals that are difficult to interpret | Number of chemical environments correctly identified |
| | Spin-Spin Coupling | No determinations made or all determinations incorrect | Some indication that spin-spin coupling determinations were used, however no systematic approach used, leading to significant errors | Systematic determination of spin-spin coupling used, however significant misinterpretations present, leading to significant errors | Systematic determination of spin-spin coupling used, however minor misinterpretations present, leading to minor errors | Splitting patterns correctly identified and number of neighbors correctly determined |
| | Integration | No determinations made or all determinations incorrect | Some indication that integration values were used, however no systematic approach used, leading to significant errors | Systematic determination of integration values used, however significant misinterpretations present, leading to significant errors | Systematic determination of integration values used, however minor misinterpretations present, leading to minor errors | Integration Values used to correctly determine the number of hydrogens giving rise to each signal |
| | Assignment | No determinations made or all determinations incorrect | Some substructure identification performed, no systematic approach used, significant major errors made in assignments | Systematic approach used in substructure identification, however significant misinterpretations present, leading to significant errors in assignments | Systematic approach used in substructure identification, however minor misinterpretations present, leading to minor errors in assignments | All chemical signals correctly interpreted into structural subunits |
| CNMR | # Chemical Environ. | No determination made | Number of chemical environments incorrectly identified, ±2 units | Minor error in determination of chemical environments, ±1 unit | Number of chemical environments determined, however determination is incorrect due to overlapping signals that are difficult to interpret | Number of chemical environments correctly identified |
| | Assignment | No determinations made or all determinations incorrect | Some substructure identification performed, no systematic approach used, significant major errors made in assignments | Systematic approach used in substructure identification, however significant misinterpretations present, leading to significant errors in assignments | Systematic approach used in substructure identification, however minor misinterpretations present, leading to minor errors in assignments | All chemical signals correctly interpreted into structural subunits |
| Analysis | Units of Unsaturation | Not found | Major error in calculation of units of unsaturation, ±2 units | Minor error in calculation of units of unsaturation, ±1 unit | Units of unsaturation determined, however a mathematical error results in an incorrect determination | Units of unsaturation correctly determined |
| | Propose Structures | No structures proposed | A single compound proposed | At least two structural isomers considered | More than two structural isomers considered | All reasonable structural isomers considered |
| | Structure determination | No analysis completed on proposed structures | Analysis performed on single compound overlooking major flaws in proposed structure leading to an incorrect determination | Analysis performed on multiple structural isomers, however major inconsistencies between spectroscopic data and proposed structures overlooked leading to an incorrect determination | Analysis performed on multiple structural isomers, however minor inconsistencies between spectroscopic data and proposed structures overlooked leading to an incorrect determination | Proposed structures analyzed to correctly determine the compound in question |