Chemistry III

Spectroscopy & Structure Determination Assignment

Date due: 4:00 p.m., Friday 23rd May 2008

Submit *via* School of Chemistry & Physics Office

Name: _____

Task: From the two sets of spectra provided, determine the structure of the unknown in each case.

You will be assessed on the accuracy and clarity of your analysis. It is NOT sufficient to simply give a structure! You MUST explain HOW you arrive at the structure and WHY you think it is correct (see the accompanying 'Guide to the Marking Criteria' for further details). Remember – if you rely on chemical shifts and/or coupling constants for the determination of your structure, you MUST prove that this information is reliable (i.e. that the spin system involved is 'First Order').

Marking Criteria – Unknown #	Max.	Unsat.	Poor	Sat.	Good	Excellent	Mark
Analysis of spectra							
Calculation of DBE's	8						
Interpretation of UV							
Interpretation of IR							
Interpretation of MS							
Interpretation of ^{1}H NMR							
Interpretation of ^{13}C NMR							
Method							
Overall approach	5						
Use of 1st Order Analysis (if required)							
Critical evaluation of proposed structure							
Structure	2						

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TOTAL MARK	*30*						

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'Guide to the Marking Criteria'

Marking Criteria & Standards	Unsat.	Poor	Sat.	Good	Excellent
Analysis of spectra					
Calculation of DBE's	Incorrect or lack of interpretation of spectroscopic and other data.	Incomplete or inappropriate interpretation of spectroscopic and other data.	Competent (minimal) interpretation of spectroscopic and other data.	Competent (detailed) interpretation of spectroscopic and other data.	Comprehensive, detailed and insightful interpretation of spectroscopic and other data.
Interpretation of UV					
Interpretation of IR					
Interpretation of MS					
Interpretation of ^{1}H NMR					
Interpretation of ^{13}C NMR					
Method					
Overall approach	No evidence shown of a systematic approach (no logical structure apparent).	Limited evidence shown of a systematic approach.	Problem is approached systematically and logically.	Problem is approached systematically and logically. Some connections made between inferences drawn from different data.	Problem is approached systematically and logically. Many, often insightful, connections made between inferences drawn from different data.
Use of 1st Order Analysis (if required)	Not applied where required.	Applied incorrectly or inappropriately.	Applied correctly.	Applied correctly and appropriate inferences drawn concerning validity of the analysis.	Applied correctly and appropriate inferences drawn concerning validity of the analysis. Possible consequences addressed.
Critical evaluation of proposed structure(s)	No explicit evaluation presented.	Limited evaluation presented.	Sufficient evaluation presented to validate (or reject) proposed structure(s).	Detailed evaluation presented to validate (or reject) proposed structure(s).	Comprehensive, detailed and insightful evaluation presented to validate (or reject) proposed structure(s).
Structure	Proposed structure is incorrect.	Proposed structure is partially correct.	Proposed structure is correct.		