THE COLLEGE OF THE BAHAMAS

EXAMINATION

SEMESTER 01-2006

FACULTY OF PURE AND APPLIED SCIENCES
SCHOOL OF SCIENCES AND TECHNOLOGY

X NASSAU
FREEPORT
EXUMA
ELEUTHERA

DATE AND TIME OF EXAMINATION: Tuesday, 19 April 2006 at 2:00 p.m.
DURATION: 3 HOURS (total for both open and closed book parts)

COURSE NUMBER: Chem 331

COURSE TITLE: Modern Structure Determination of Organic Compounds

STUDENT NAME:

STUDENT NUMBER:

LECTURER'S NAME: Dr. D. Davis

INSTRUCTIONS TO CANDIDATES:

This examination paper consists of 8 questions on 4 pages (excluding this instruction page). Answer ALL questions in the spaces provided on the examination paper. Students are allowed to use calculators during this examination.

This is the **CLOSED BOOK** portion of this final exam.

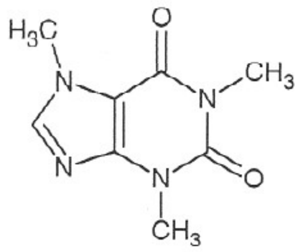
Upon completion of this portion of the exam you are required to complete the open book portion of this examination.

PERIODIC TABLE OF THE ELEMENTS

I	II											III	IV	V	VI	VII	0
1 H hydrogen 1·0																	2 He helium 4·0
3 Li lithium 6·9	4 Be beryllium 9·0											5 B boron 10·8	6 C carbon 12·0	7 N nitrogen 14·0	8 O oxygen 16·0	9 F fluorine 19·0	10 Ne neon 20·2
11 Na sodium 23·0	12 Mg magnesium 24·3											13 Al aluminium 27·0	14 Si silicon 28·1	15 P phosphorus 31·0	16 S sulfur 32·1	17 Cl chlorine 35·5	18 Ar argon 39·9
19 K potassium 39·1	20 Ca calcium 40·1	21 Sc scandium 45·0	22 Ti titanium 47·9	23 V vanadium 50·9	24 Cr chromium 52·0	25 Mn manganese 54·9	26 Fe iron 55·8	27 Co cobalt 58·9	28 Ni nickel 58·7	29 Cu copper 63·5	30 Zn zinc 65·4	31 Ga gallium 69·7	32 Ge germanium 72·6	33 As arsenic 74·9	34 Se selenium 79·0	35 Br bromine 79·9	36 Kr krypton 83·8
37 Rb rubidium 85·5	38 Sr srontium 87·6	39 Y yttrium 88·9	40 Zr zirconium 91·2	41 Nb niobium 92·9	42 Mo molybdenum 95·9	43 Tc technetium 98·9	44 Ru ruthenium 101·1	45 Rh rhodium 102·9	46 Pd paladium 106·4	47 Ag silver 107·9	48 Cd cadmium 112·4	49 In indium 114·8	50 Sn tin 118·7	51 Sb antimony 121·8	52 Te tellurium 127·6	53 I iodine 126·9	54 Xe xenon 131·3
55 Cs cesium 132·9	56 Ba barium 137·3	57 La lanthanum 138·9	72 Hf hafnium 178·5	73 Ta tantalum 180·9	74 W tungsten 183·85	75 Re rhenium 186·2	76 Os osmium 190·2	77 Ir iridium 192·2	78 Pt platinum 195·1	79 Au gold 197·0	80 Hg mercury 200·6	81 Tl thallium 204·4	82 Pb lead 207·2	83 Bi bismuth 209·0	84 Po polonium	85 At astaline	86 Rn radon
87 Fr francium	88 Ra radium	89 Ac actinium															

58 Ce cerium	59 Pr praseodymium	60 Nd neodymium	61 Pm promethium	62 Sm samarium	63 Eu europium	64 Gd gadolinium	65 Tb terbium	66 Dy dysprosium	67 Ho holmium	68 Er erbium	69 Tm thulium	70 Yb ytterbium	71 Lu lutetium
90 Th thorium	91 Pa protoactinium	92 U uranium	93 Np neptunium	94 Pu plutonium	95 Am americium	06 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

1. A chemist isolated a sample, believed to be caffeine, from tea leaves. An elemental analysis of the white solid gave the following composition: C(49.48%) H(5.19%) N(28.85%) O(16.48%).

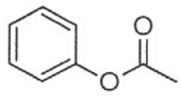


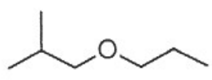
(a) What is the empirical formula of the unknown?

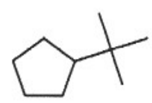
(b) Does the elemental analysis support the hypothesis that the solid is caffeine?

[6 marks]

2. Predict the total number of unique proton nmr **and** carbon nmr absorptions in each of the following compounds. You are NOT required to estimate the chemical shift of the signals.

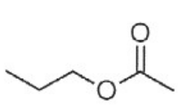
(a) 

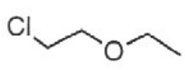
(b) 

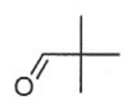
(c) 

[6 marks]

3. Predict the spin-spin splitting pattern **and** integration for each unique proton resonance in the following molecules:

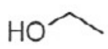
(a) 

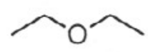
(b) 

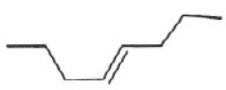
(c) 

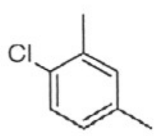
[6 marks]

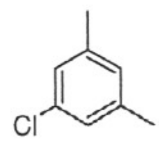
4. What spectrometric technique (ir, ms, ^{1}H or ^{13}C nmr) is best suited to ascertain the difference between the following pairs of compounds? You are only allowed to use each technique once in this question. State generally what difference(s) you expect to observe in the spectral technique chosen.

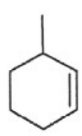
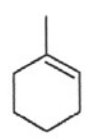
(a) 

vs 

(b)  *vs* 

(c) 

vs 

(d)  *vs* 

[8 marks]

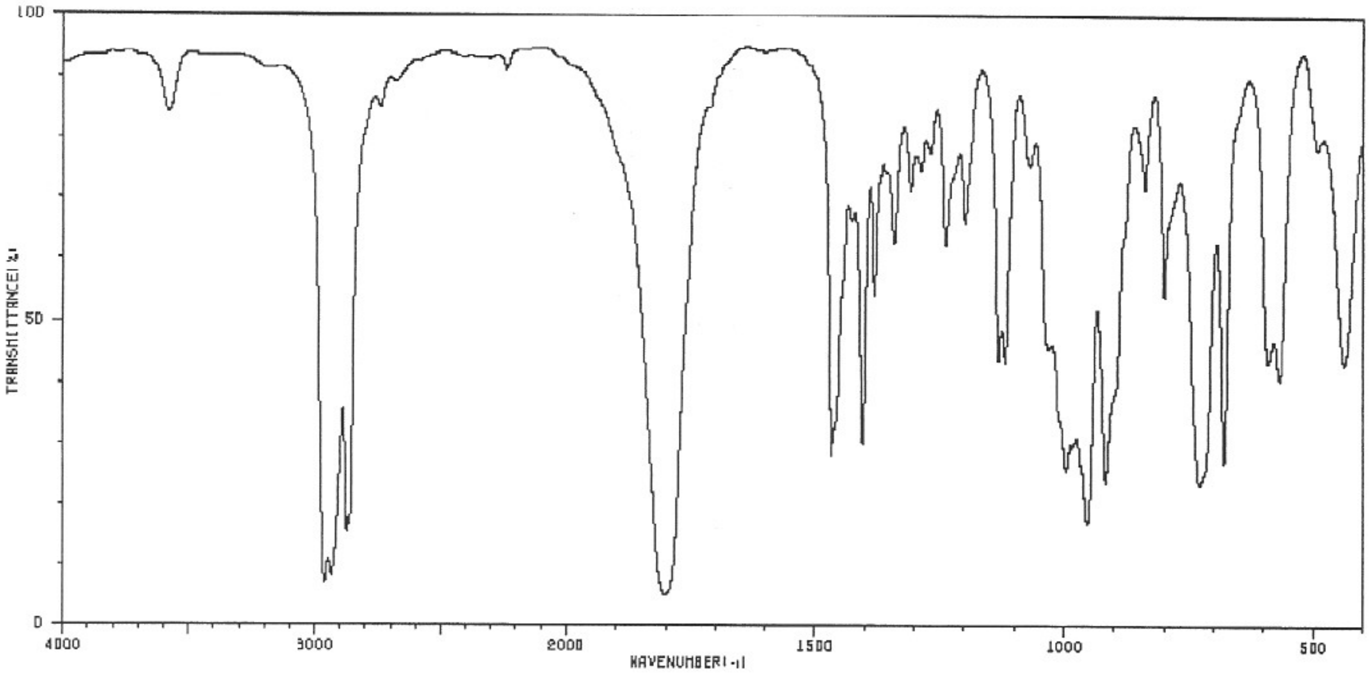
5. What is the origin of the M+1 and the M+2 peak of 1-chlorodecanoic acid?

[4 marks]

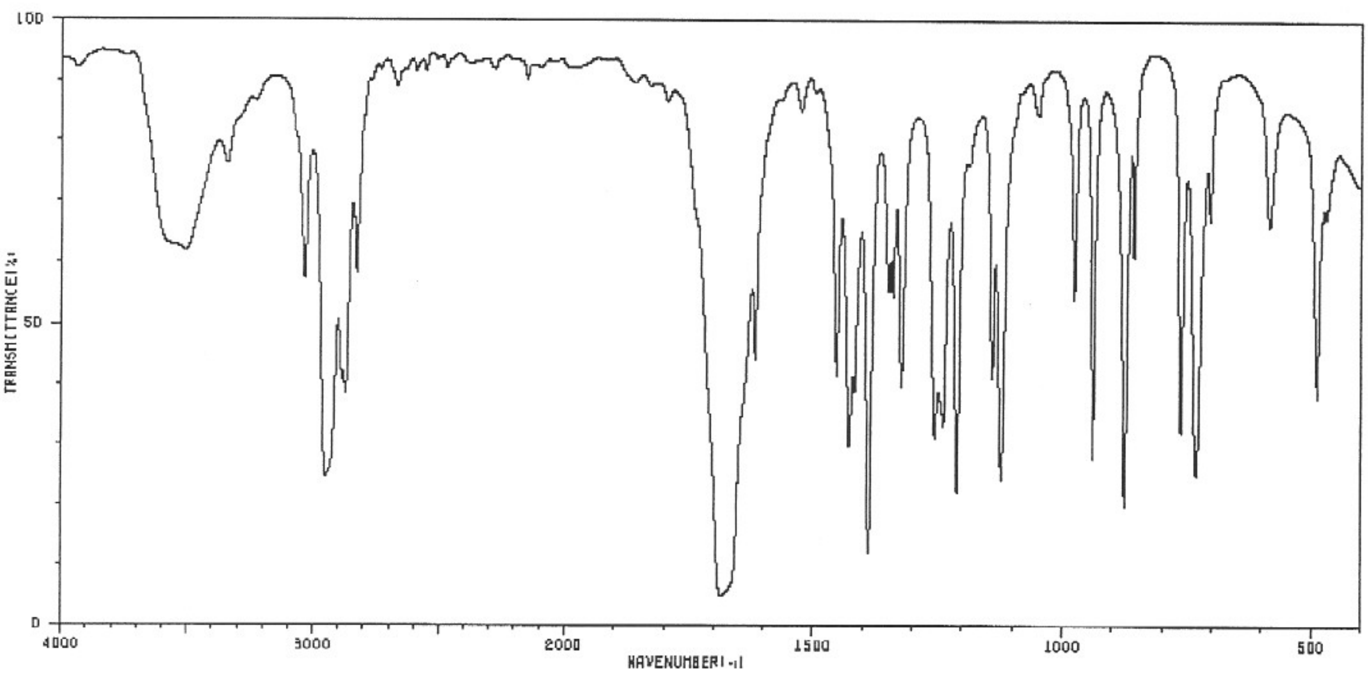
6. Explain the origin and intensity of a triplet in a ^{1}H nmr spectrum. A diagram and a few words may provide your best approach to answering this question.

[3 marks]

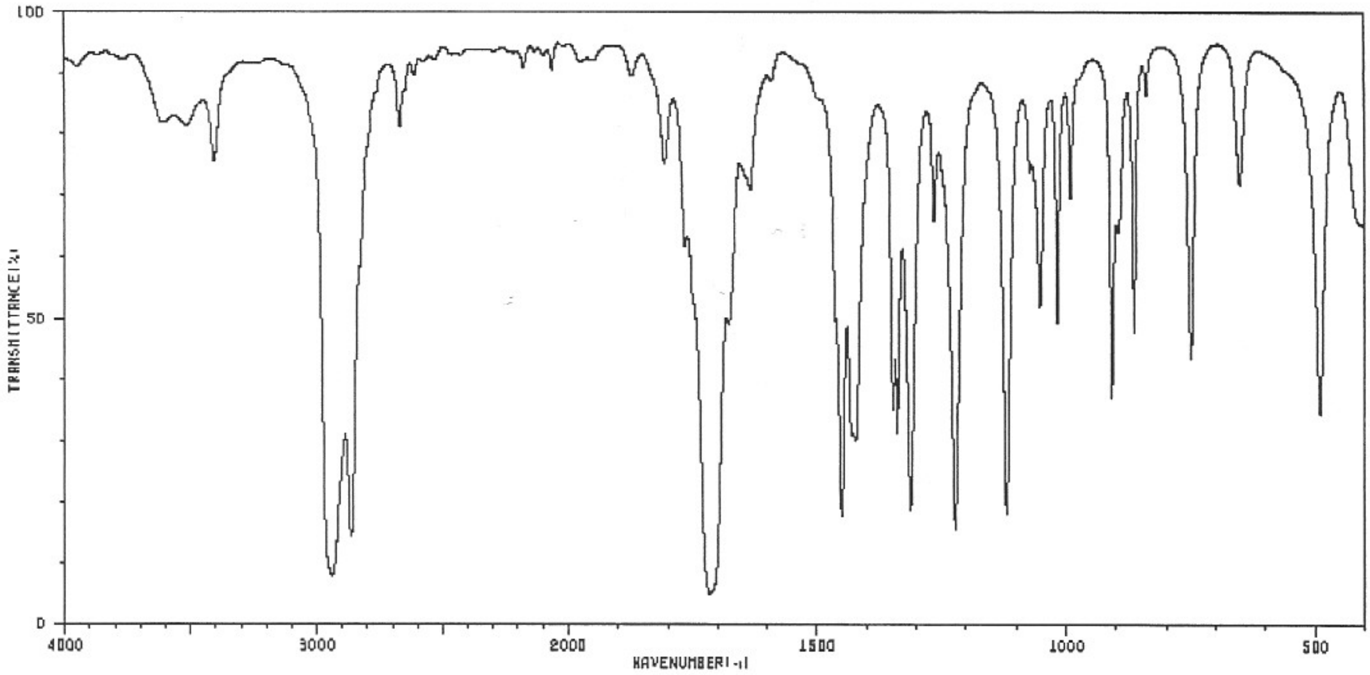
7. The ir spectra of hexanoylchloride, cyclohexanone and cyclohexen-1-one are shown below. Assign each compound to its respective spectrum. A full analysis of the spectrum is not required just state a reason for each assignment.



3680	81	1468	26	1288	72	997	24	692	42
2961	6	1461	31	1269	74	955	16	584	43
2935	7	1427	64	1239	80	918	22	577	42
2876	14	1406	28	1199	64	840	68	569	38
2864	15	1381	52	1132	42	801	52	491	74
2739	81	1342	60	1119	42	730	22	438	41
1800	4	1308	68	1069	72	680	26		



3341	72	1796	84	1388	11	1141	39	868	68
3034	55	1685	4	1349	53	1123	23	763	31
2951	23	1617	42	1340	52	1056	84	733	23
2887	38	1626	81	1324	38	1048	81	706	64
2871	36	1454	39	1257	30	977	52	586	64
2829	55	1428	28	1240	32	940	26	489	36
2670	86	1417	37	1212	21	876	18	472	64



3610	79	2611	86	1460	17	1222	16	896	62
3515	79	1870	86	1429	30	1119	17	864	46
3407	72	1808	72	1422	28	1073	72	839	64
2941	7	1766	60	1347	34	1062	60	760	42
2864	13	1716	4	1338	30	1018	47	652	70
2870	79	1677	47	1311	17	991	68	490	33
2654	84	1634	68	1265	64	909	36		

[6 marks]

8. Methyl hexanoate and ethyl pentanoate can be distinguished from each other by examining the McLafferty rearrangement products.

(a) Show the mechanism for the formation of the McLafferty rearrangement product of each compound.

(b) Calculate the mass of the ion observed for the McLafferty rearrangement product for each of these two compounds.

[6 marks]

******** End of Examination ********