CHEMISTRY 3331: Fundamentals of Organic Chemistry I

Prof. Ognjen Š. Miljanić

Final Exam

December 6, 2016

Name: Answer Key

(print legibly) Last First

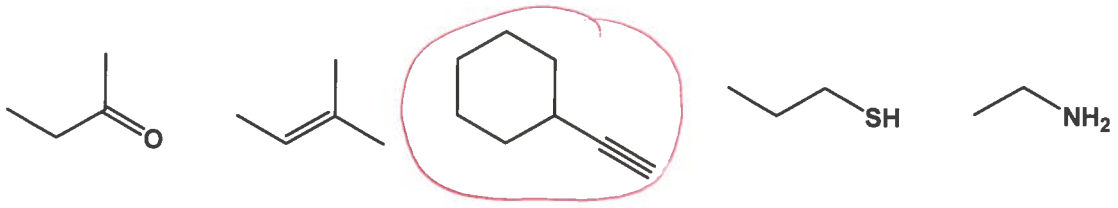
Student ID Number: N/A

Read all directions very carefully. Write your answer legibly in the designated spaces. Total number of points is 300. This exam is printed on both sides and should have six pages.

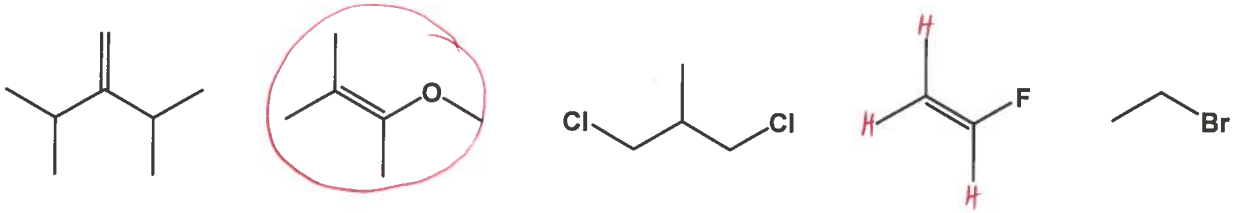
20

1. This question has several parts. In each, **circle only one entry.**

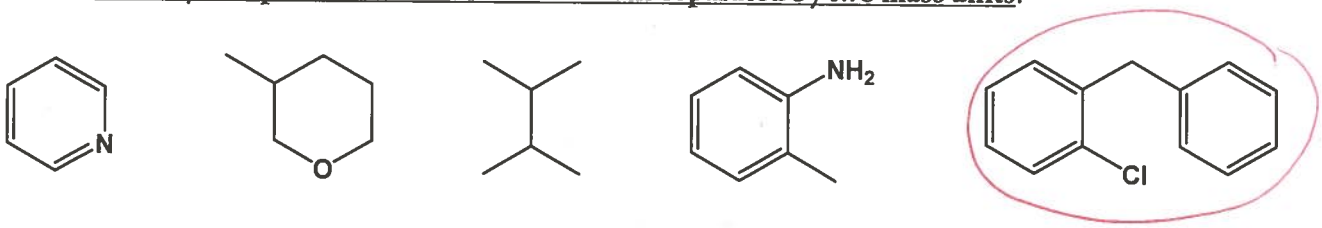
Circle the only compound that will have an IR band* at approx. 3300 cm^{-1}: *4 × 5 = 20 points*



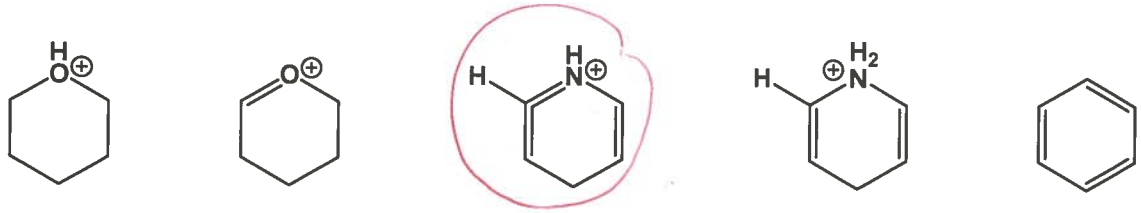
Circle the only compound that will show only singlets in its ^{1}H NMR spectrum:



Circle the only compound with two molecular ions separated by two mass units:



Circle the only meaningless structure:



* Detailed information on IR bands of different functional groups can be found at http://www2.ups.edu/faculty/hanson/Spectroscopy/IR/IRfrequencies.html

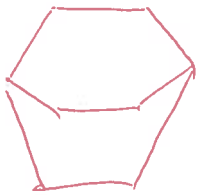
DO NOT WRITE IN THIS SPACE

300

FINAL SCORE

20

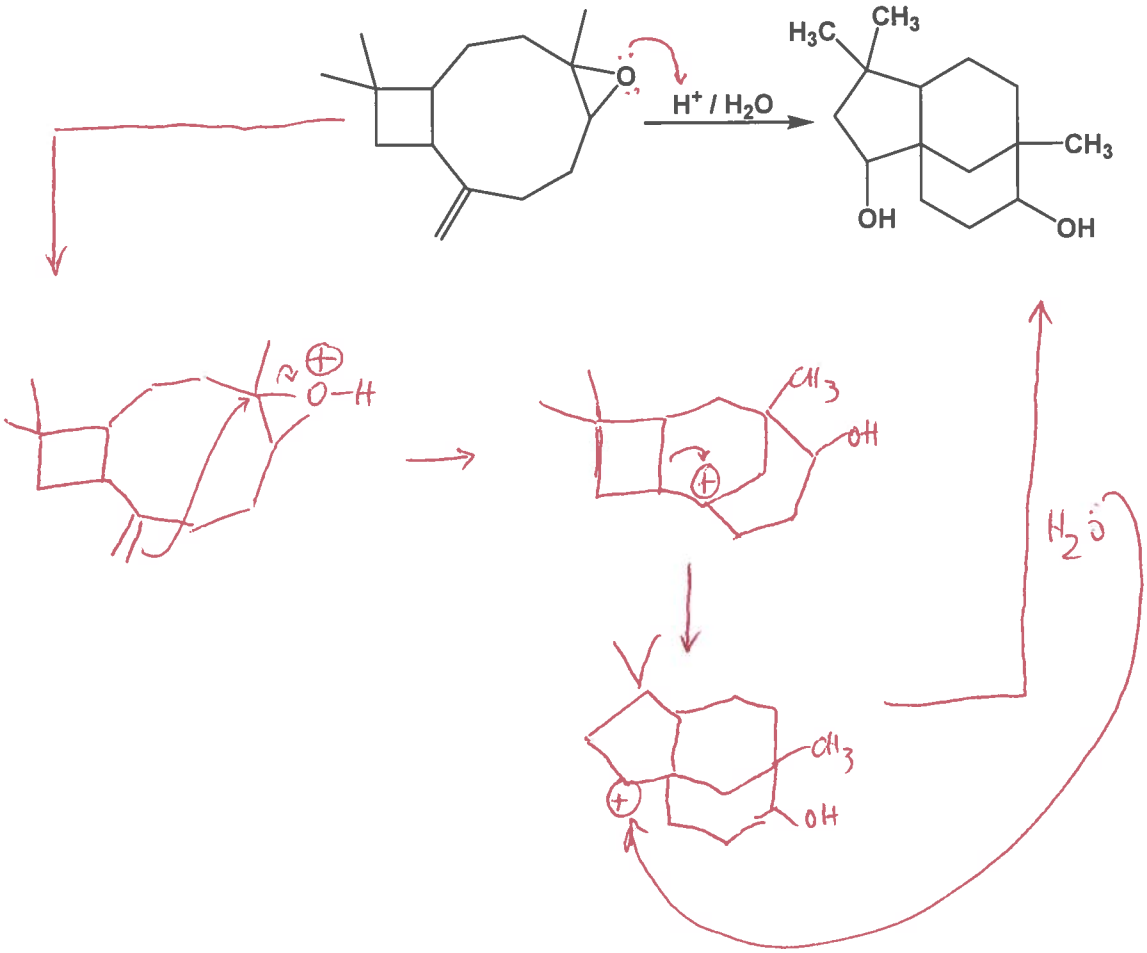
2. Normally, the chair conformation of cyclohexane is more stable than its boat conformation. But sometimes (rarely) this relationship switches and the boat conformation becomes more stable. Propose an example of a molecule in which this may happen and explain why. *20 points*



ring strain forces this molecule into a boat conformation

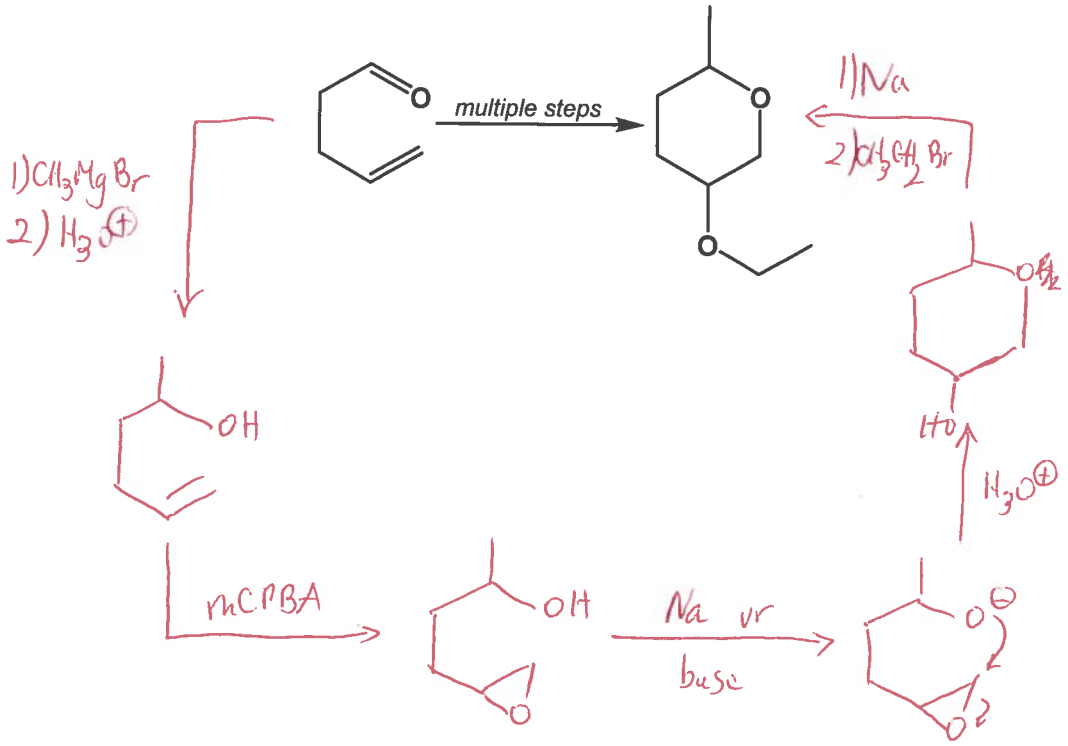
30

3. Propose a reasonable mechanism for the transformation shown below, using curved arrows to indicate the flow of electrons. Do not draw transition states. *30 points*



50

4. Propose a sequence of synthetic steps that would efficiently accomplish the conversion shown below. You can use any inorganic reagents you want, and organic reagents with two carbon atoms or less. Show all starting materials and necessary reagents, but do not give mechanisms. *50 points*



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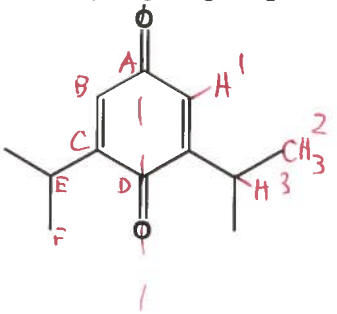
5. Predict the ^1H spectrum of the compound shown below. Give the following information: (*a*) number of peaks that will be observed; (*b*) integrated area of those peaks, and (*c*) peak multiplicity, also known as peak splitting (e.g. singlet, quartet). How many peaks would you expect in its ^{13}C NMR spectrum? *40 points*



a) 3 peaks

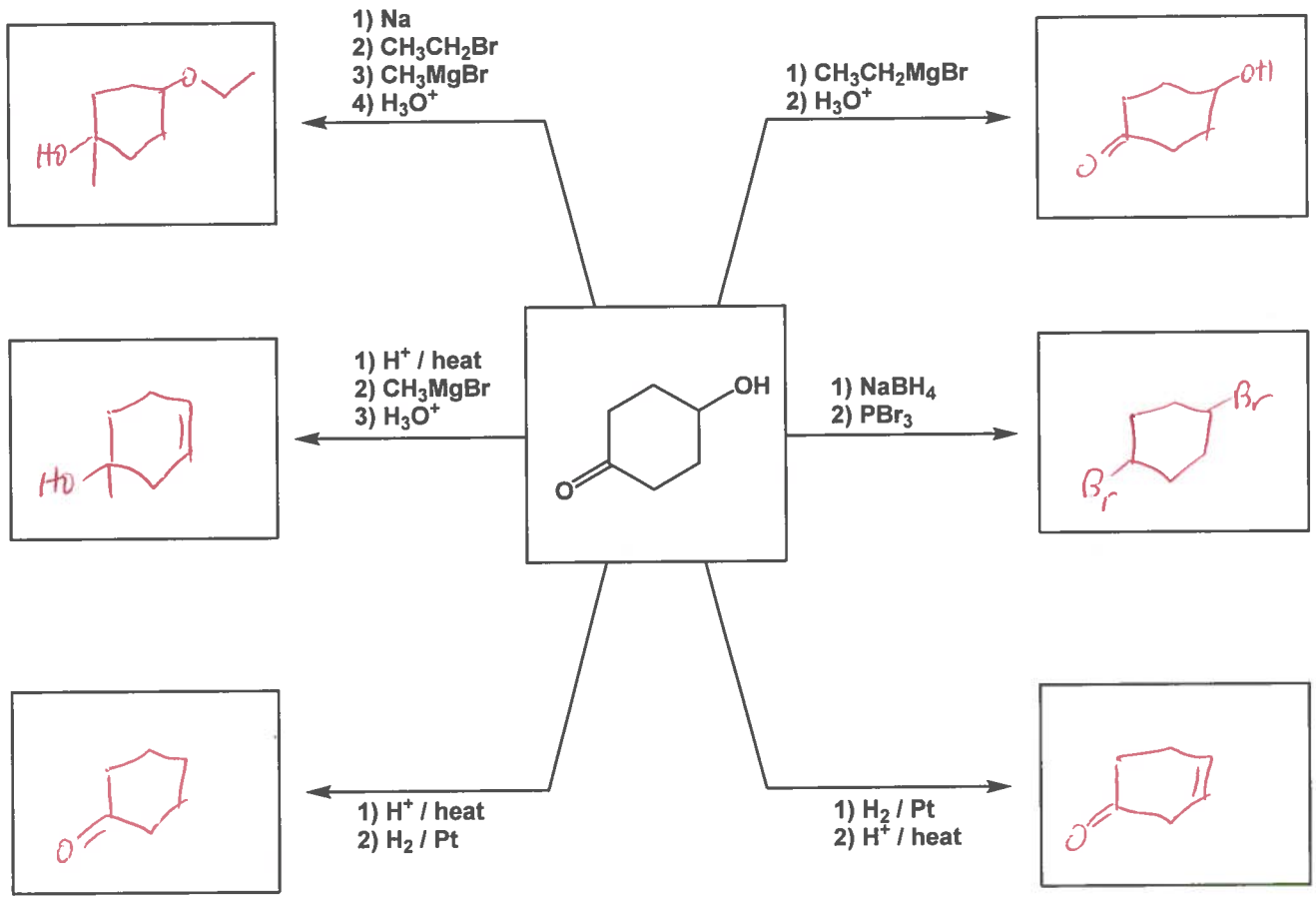
b) 2 : 2 : 12

c) 1: singlet
2: doublet
3: septet (7 peaks)

6 peaks in ^{13}C NMR: A–F

60

6. Write the products of the reactions of the compound shown in the center with the reagents shown on the arrows. Make sure to include stereochemistry, but do not write mechanisms. *60 points*



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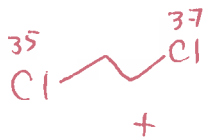
7. Predict how the mass spectrum of 1,2-dichloroethane would look like. Specify the number of molecular ions that you would observe, their masses, and their relative ratios. *20 points*

98 g/mol

Likelihood

$3/4 \times 3/4 = 9/16$



+

100 g/mol

Likelihood

$\left(\frac{3}{4} \times \frac{1}{4}\right) + \left(\frac{1}{4} \times \frac{3}{4}\right) = \frac{6}{16}$

102 g/mol

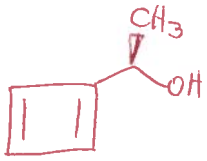
Likelihood

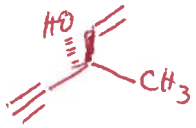
$\frac{1}{4} \times \frac{1}{4} = \frac{1}{16}$

ratio 9:6:1

15

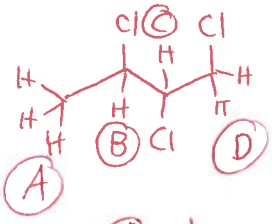
8. Draw an example of a chiral molecule with a molecular formula C_6H_8O. *15 points*



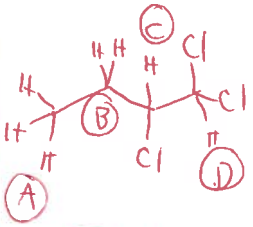


15

9. Explain how splitting of peaks in the ^{1}H NMR spectra of 1,2,3-trichlorobutane and 1,1,2-trichlorobutane can be used to distinguish these two compounds. *15 points*



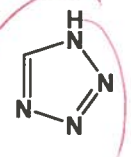
A: d, 3H
B: dq, 1H
C: dt, 1H
D: d, 2H

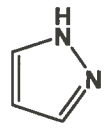


A: ~~d~~ t, 3H
B: dq, 2H
C: dt, 1H
D: d, 2H

30

10. Tetrazole (shown on the left) has a pK_a of 4.9, while pyrazole (right) has a pK_a of 11.5. Circle the stronger acid. Then, explain the difference in acidity using resonance structures. *30 points*

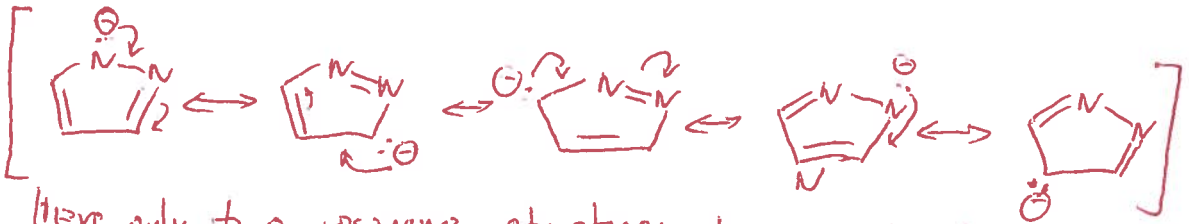

tetrazole


pyrazole

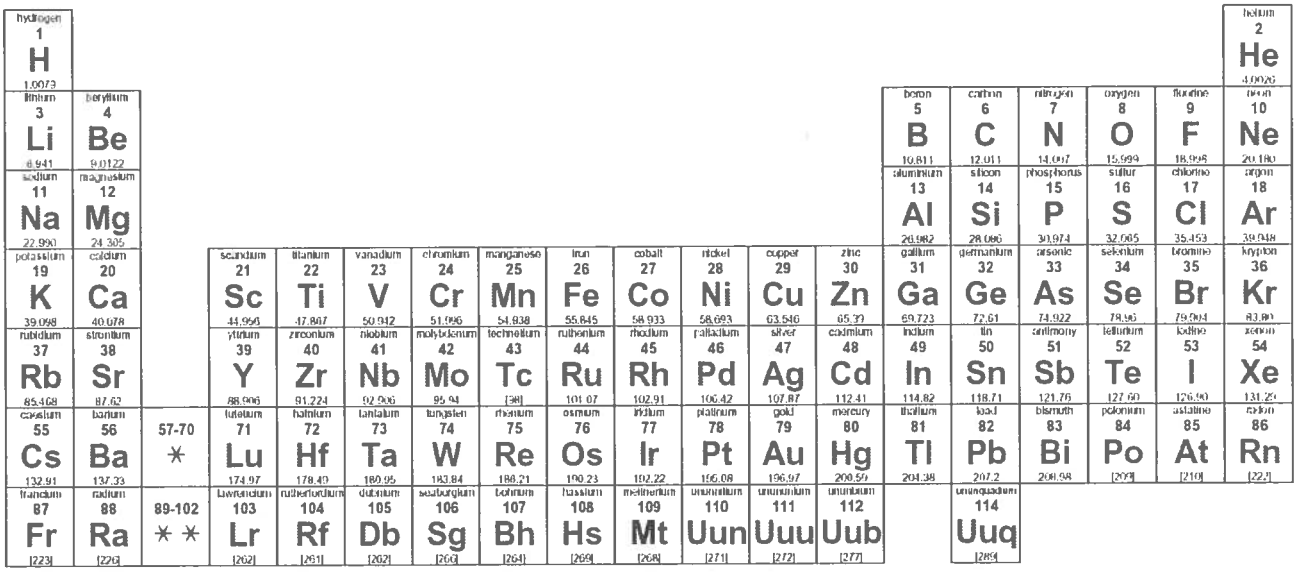
Stronger acid

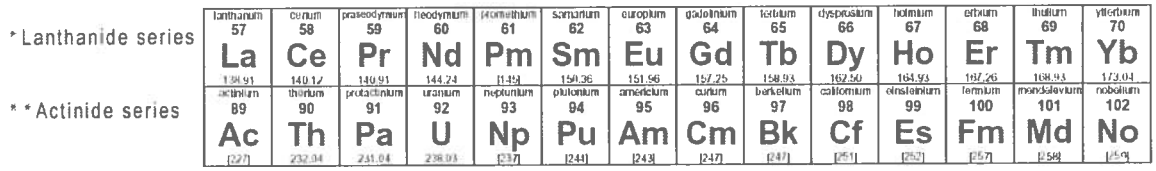
Deprotonation gives these two anions:

in all but one resonance structure, ⊖ is on N - an electronega-tive atom



Here, only two resonance structures have a ⊖ charge on nitrogen - in others, it is on electropositive carbon


hydrogen 1 H 1.0079
helium 2 He 4.0026
lithium 3 Li 6.941
beryllium 4 Be 9.0122
boron 5 B 10.811
carbon 6 C 12.011
nitrogen 7 N 14.007
oxygen 8 O 15.999
fluorine 9 F 18.998
neon 10 Ne 20.180
sodium 11 Na 22.990
magnesium 12 Mg 24.305
aluminium 13 Al 26.982
silicon 14 Si 28.086
phosphorus 15 P 30.974
sulfur 16 S 32.065
chlorine 17 Cl 35.453
argon 18 Ar 39.948
potassium 19 K 39.098
calcium 20 Ca 40.078
scandium 21 Sc 44.956
titanium 22 Ti 47.867
vanadium 23 V 50.942
chromium 24 Cr 51.996
manganese 25 Mn 54.938
iron 26 Fe 55.845
cobalt 27 Co 58.933
nickel 28 Ni 58.693
copper 29 Cu 63.546
zinc 30 Zn 65.39
gallium 31 Ga 69.723
germanium 32 Ge 72.61
arsenic 33 As 74.922
selenium 34 Se 78.96
bromine 35 Br 79.904
krypton 36 Kr 83.80
rubidium 37 Rb 85.468
strontium 38 Sr 87.62
yttrium 39 Y 88.906
zirconium 40 Zr 91.224
niobium 41 Nb 92.906
molybdenum 42 Mo 95.94
technetium 43 Tc [98]
ruthenium 44 Ru 101.07
rhodium 45 Rh 102.91
palladium 46 Pd 106.42
silver 47 Ag 107.87
cadmium 48 Cd 112.41
indium 49 In 114.82
tin 50 Sn 118.71
antimony 51 Sb 121.76
tellurium 52 Te 127.60
iodine 53 I 126.90
xenon 54 Xe 131.29
caesium 55 Cs 132.91
barium 56 Ba 137.33
57-70 *
lutetium 71 Lu 174.97
hafnium 72 Hf 178.49
tantalum 73 Ta 180.95
tungsten 74 W 183.84
rhenium 75 Re 186.21
osmium 76 Os 190.23
iridium 77 Ir 192.22
platinum 78 Pt 195.08
gold 79 Au 196.97
mercury 80 Hg 200.59
thallium 81 Tl 204.38
lead 82 Pb 207.2
bismuth 83 Bi 208.98
polonium 84 Po [209]
astatine 85 At [210]
radon 86 Rn [222]
francium 87 Fr [223]
radium 88 Ra [226]
89-102 * *
lawrencium 103 Lr [262]
rutherfordium 104 Rf [261]
dubnium 105 Db [262]
seaborgium 106 Sg [266]
bohrium 107 Bh [264]
hassium 108 Hs [269]
meitnerium 109 Mt [268]
ununnilium 110 Uun [271]
unununium 111 Uuu [272]
ununbium 112 Uub [277]
ununquadium 114 Uuq [289]


* Lanthanide series
* * Actinide series
lanthanum 57 La 138.91
cerium 58 Ce 140.12
praseodymium 59 Pr 140.91
neodymium 60 Nd 144.24
promethium 61 Pm [145]
samarium 62 Sm 150.36
europium 63 Eu 151.96
gadolinium 64 Gd 157.25
terbium 65 Tb 158.93
dysprosium 66 Dy 162.50
holmium 67 Ho 164.93
erbium 68 Er 167.26
thulium 69 Tm 168.93
ytterbium 70 Yb 173.04
actinium 89 Ac [227]
thorium 90 Th 232.04
protactinium 91 Pa 231.04
uranium 92 U 238.03
neptunium 93 Np [237]
plutonium 94 Pu [244]
americium 95 Am [243]
curium 96 Cm [247]
berkelium 97 Bk [247]
californium 98 Cf [251]
einsteinium 99 Es [252]
fermium 100 Fm [257]
mendelevium 101 Md [258]
nobelium 102 No [259]