

50 points

Due last class

You must propose and defend a structure for compounds 1-5 (ten points apiece). In addition to the structure proposal, you must interpret the data in the spectra provided. Specifically, for the IR spectrum you must assign three absorbances to functional groups in the molecule and you must assign each peak in the ^1H NMR spectrum to a proton in the molecule and each peak in the ^{13}C NMR spectrum to a carbon in the molecule.

For each compound you are provided a molecular formula, IR, ^1H NMR, and ^{13}C NMR spectrum and either a MS or the molecular formula. In the ^1H NMR, integrations are provided between the spectrum and frequency scale. Multiplicity splittings are indicated on the spectrum according the following legend: s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet. Other splittings are indicated by combining these or are written out. If an asterisk is included (e.g. s*) the signal exchanges with D_2O (i.e. when D_2O is added to the NMR sample, the indicated signal disappears from the spectrum. This indicates that the proton in question is either on an OH or NH.

Work must be shown. Some partial credit will be awarded for incorrect structures with good analysis shown.

In addition to your proposed structure, show:

Molecular formula: unsaturations in molecule

IR spectrum: assign three absorbances to functional groups in molecule

^1H NMR: assign each signal to a proton(s) in the molecule

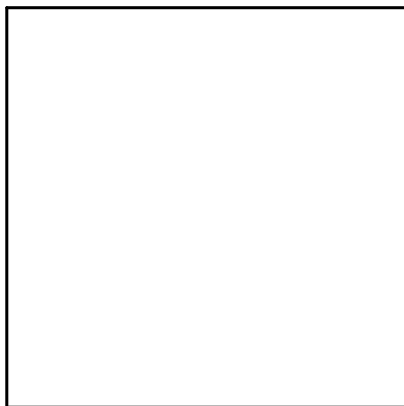
^{13}C NMR: assign each signal to a carbon(s) in the molecule

You may find it useful to look at some of the spectra electronically – magnifying the peaks may shed light on coupling.

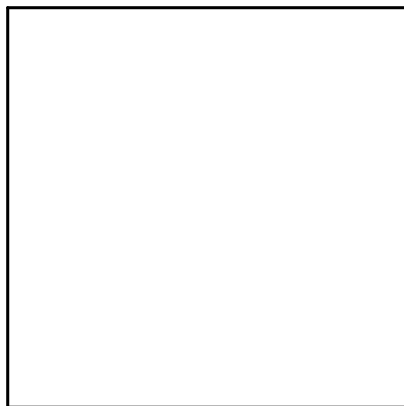
You may use your text, class and lab notes and other study partners currently enrolled in Chm 123. No other help or aid is allowed.

Draw your assigned structure neatly in the box:

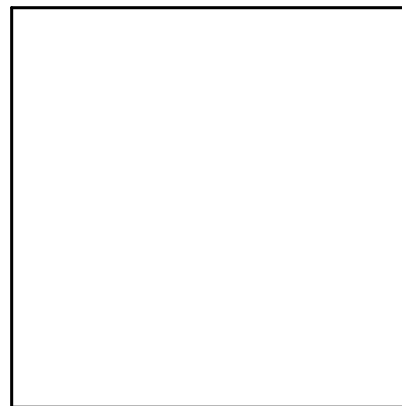
Compound 1



2



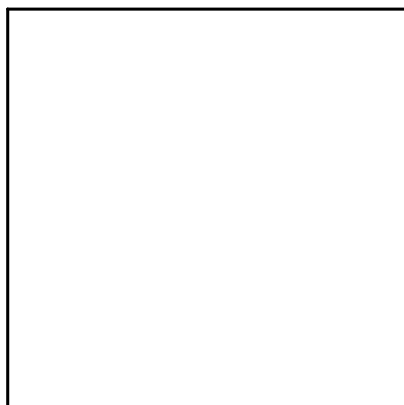
3



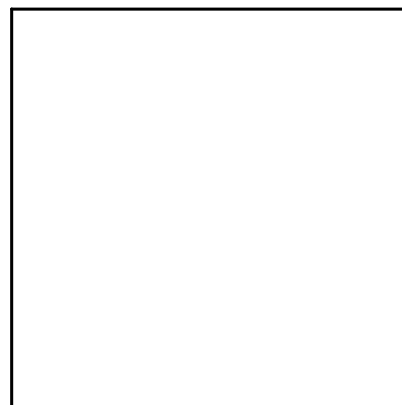
Compound 4



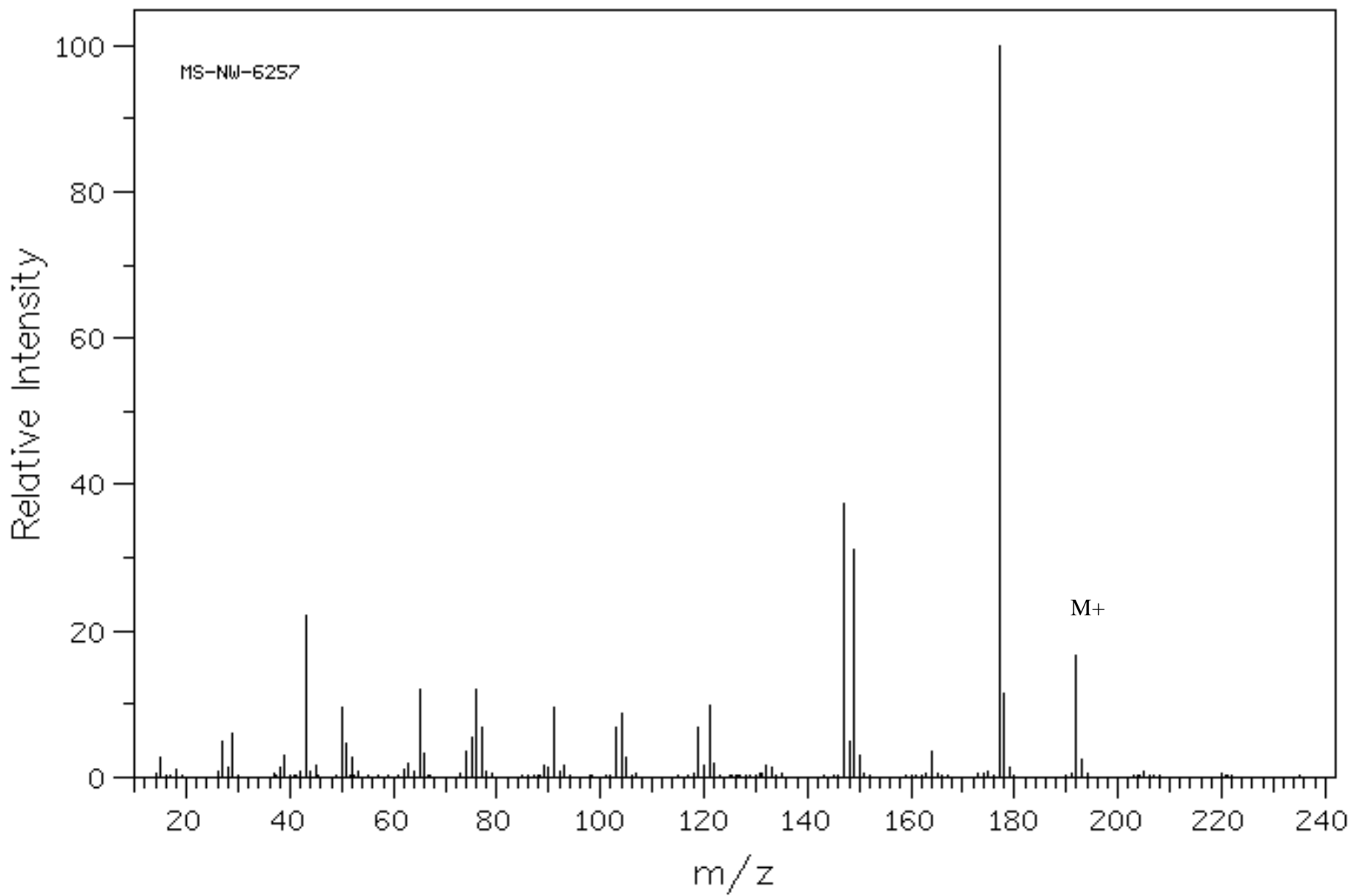
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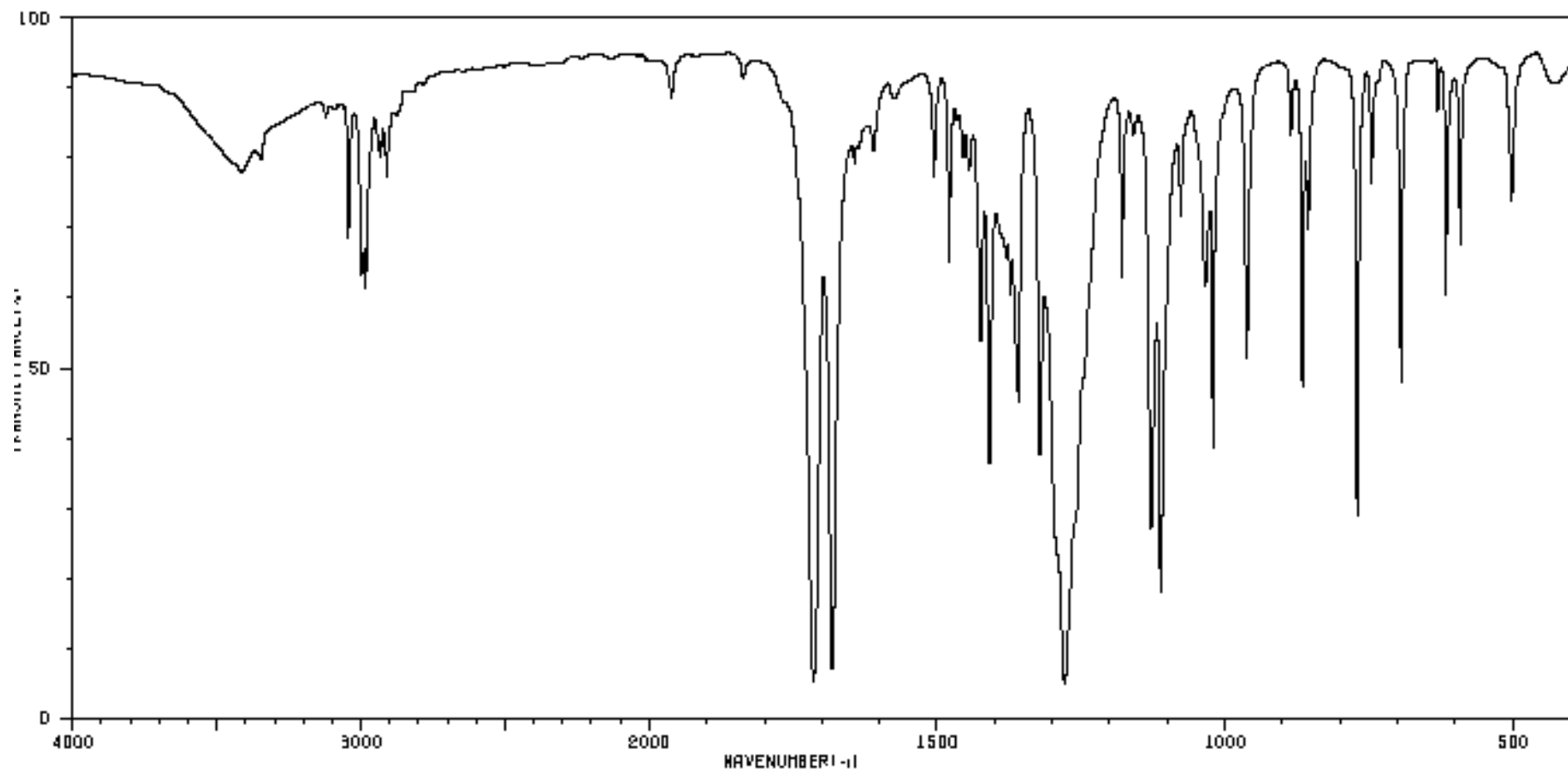


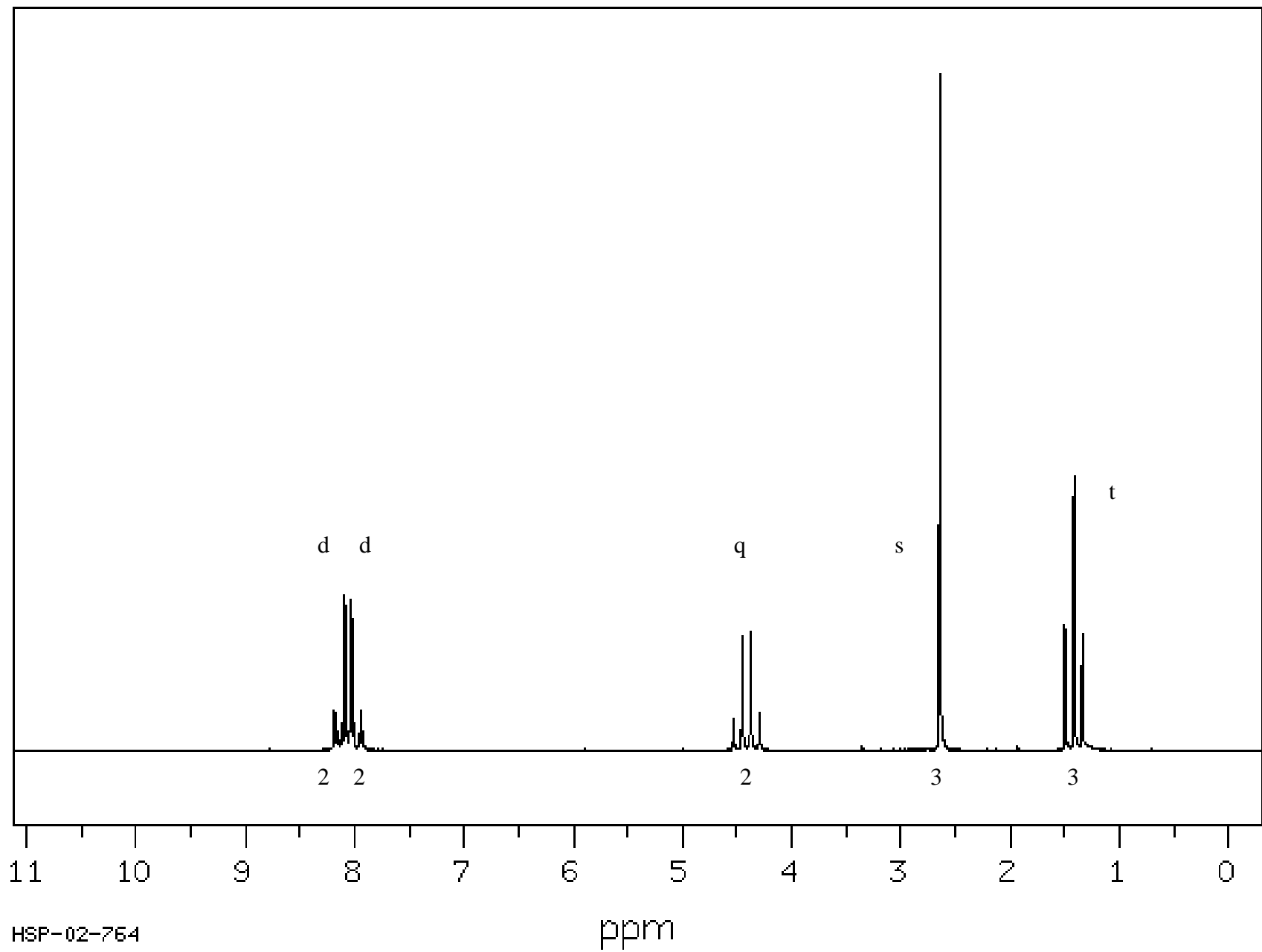
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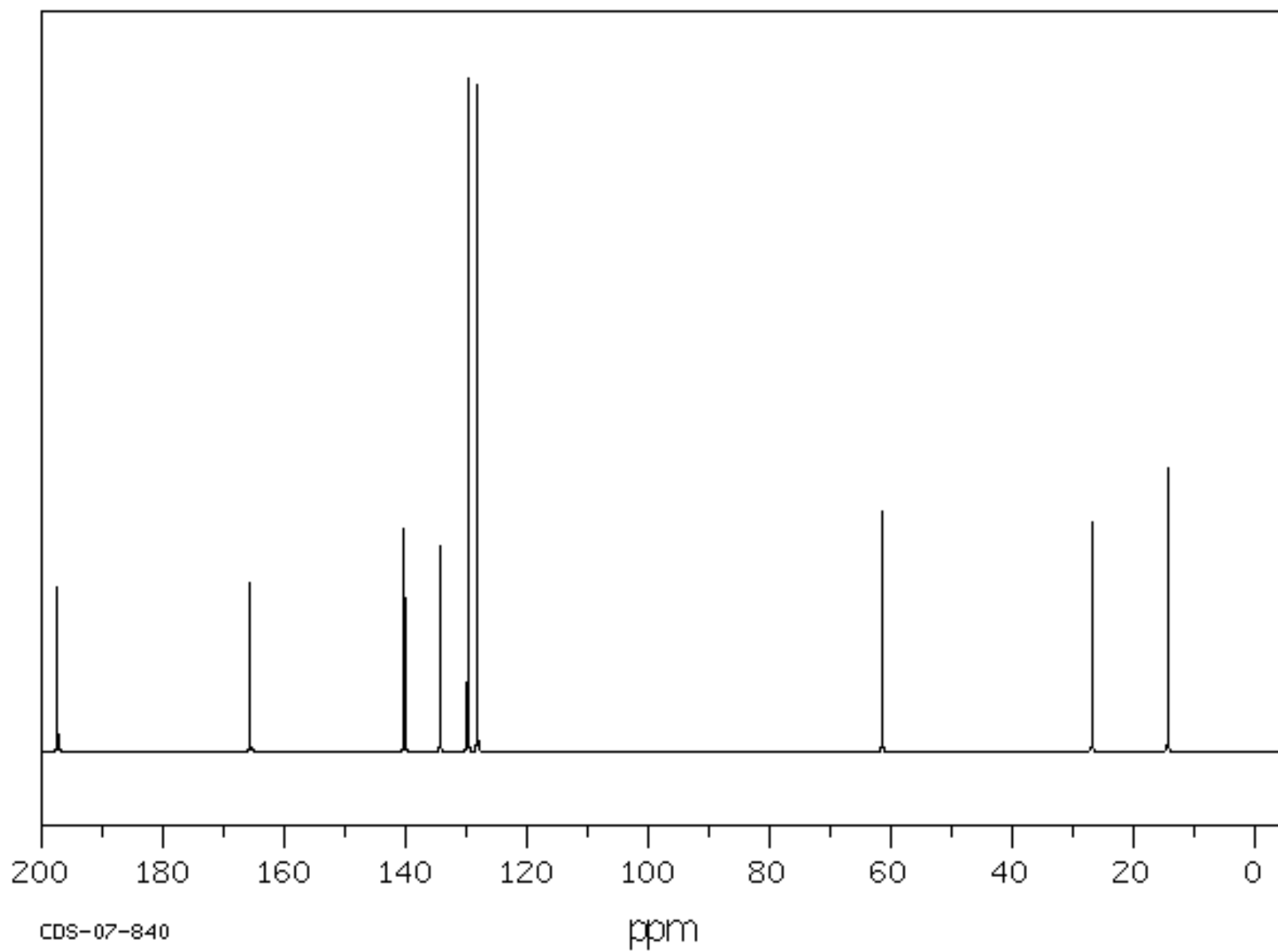
1.



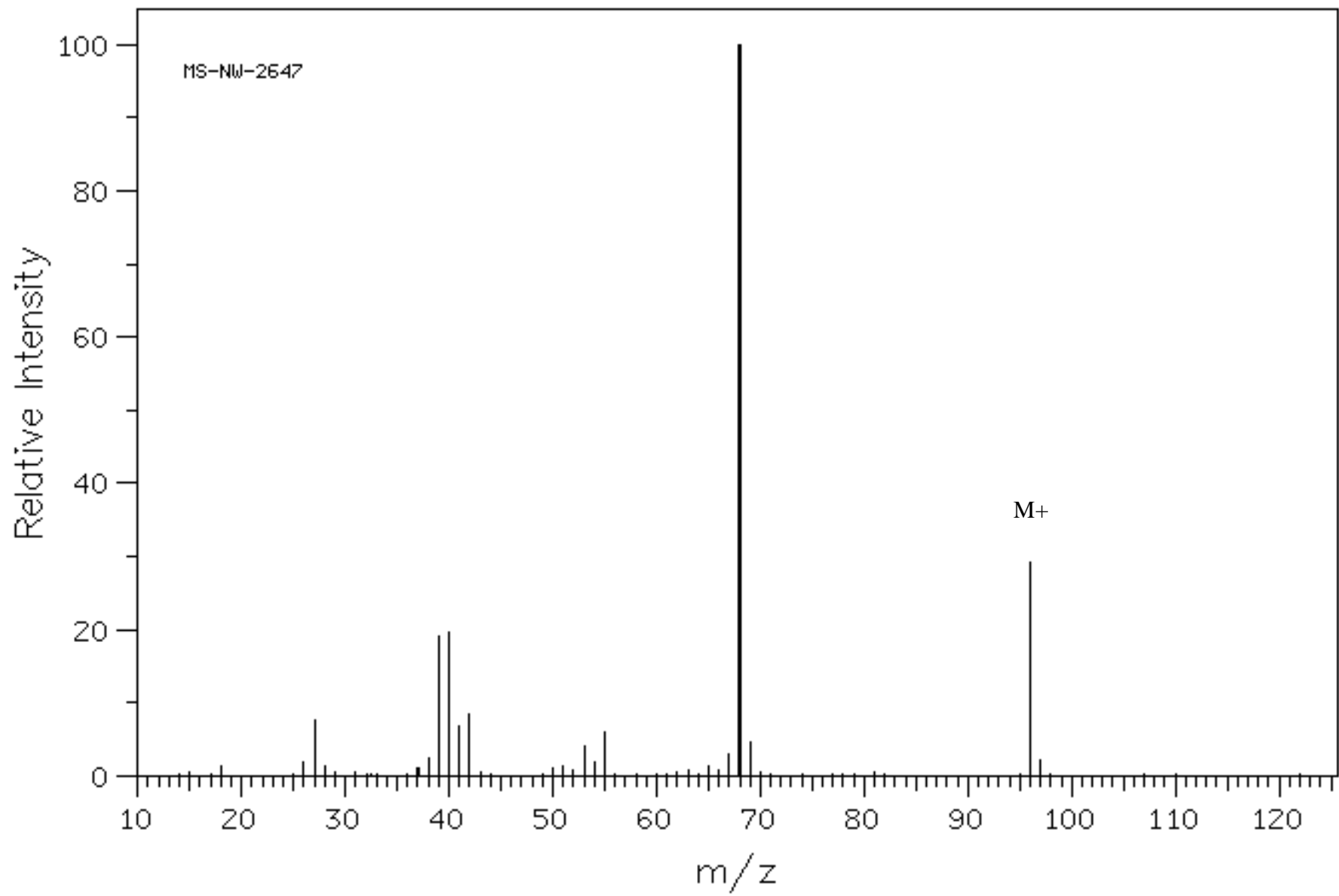


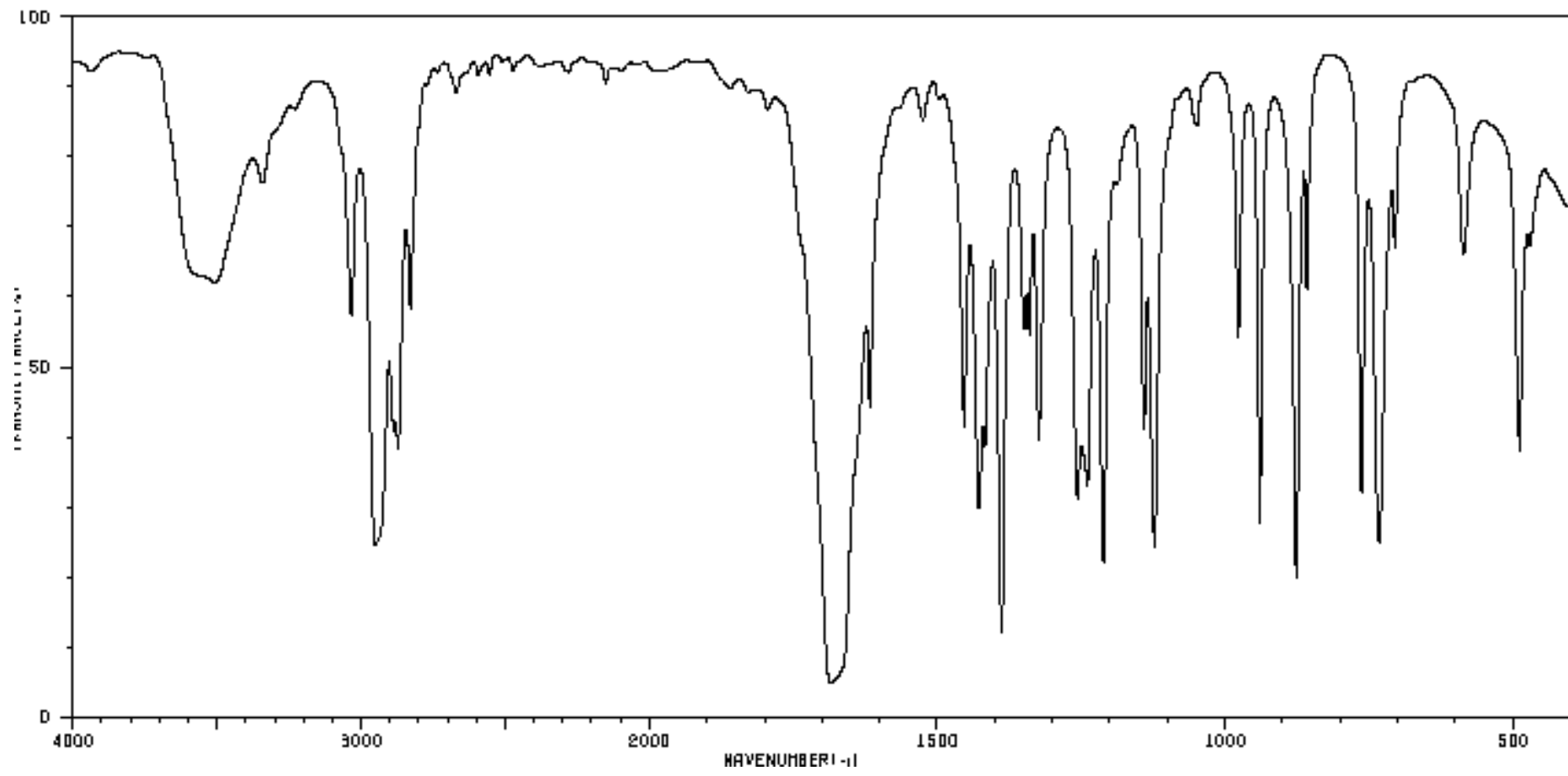


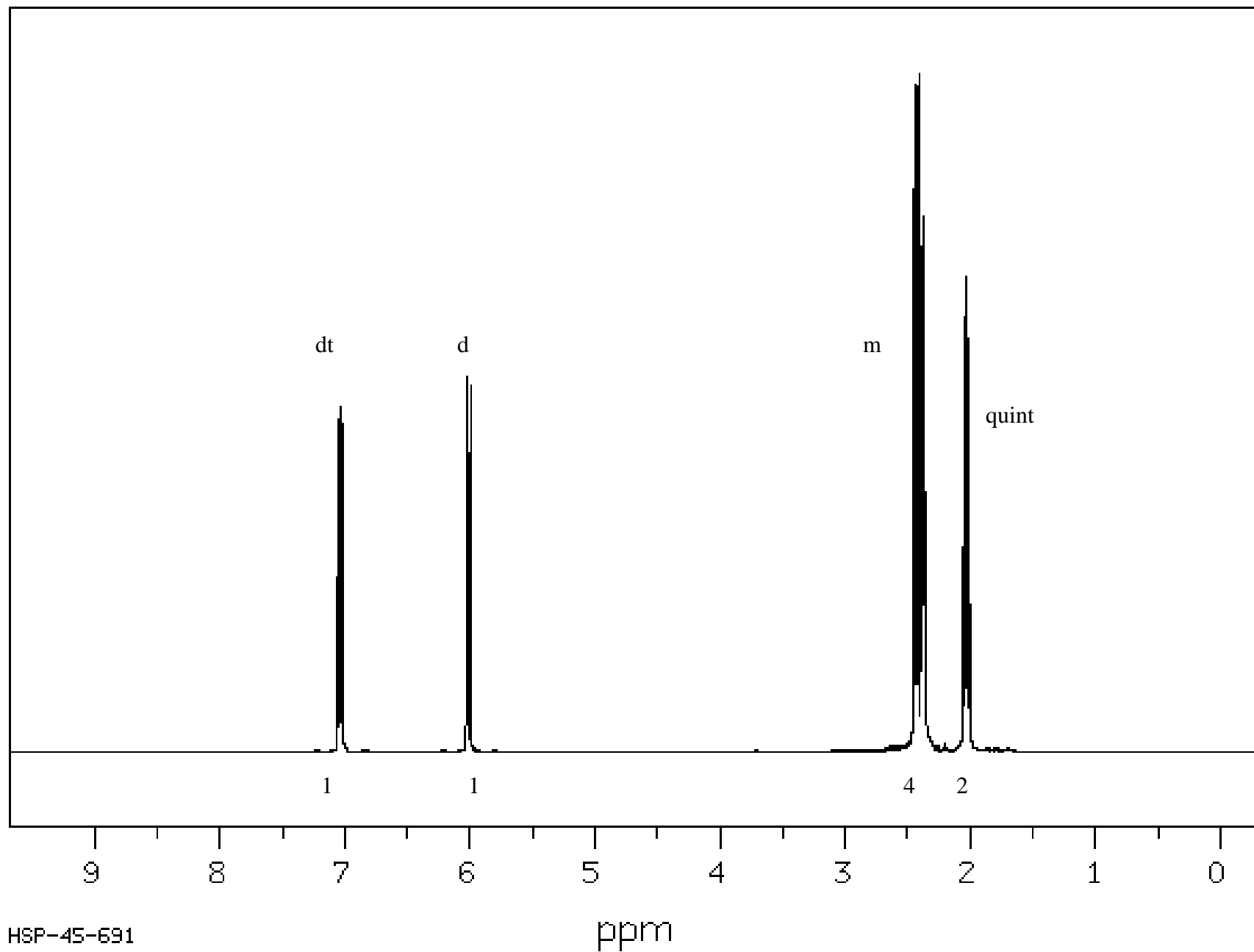
HSP-02-764



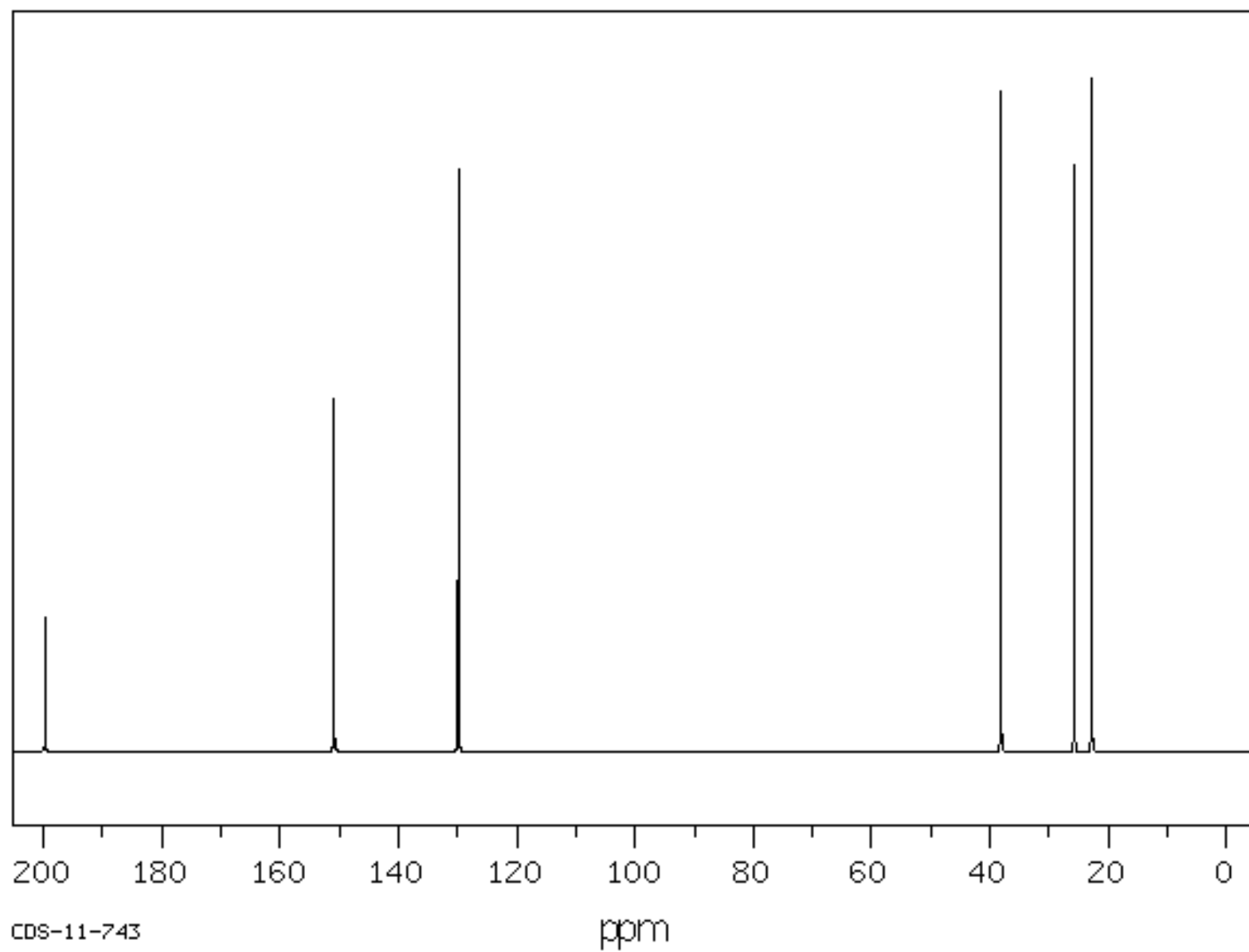
2.



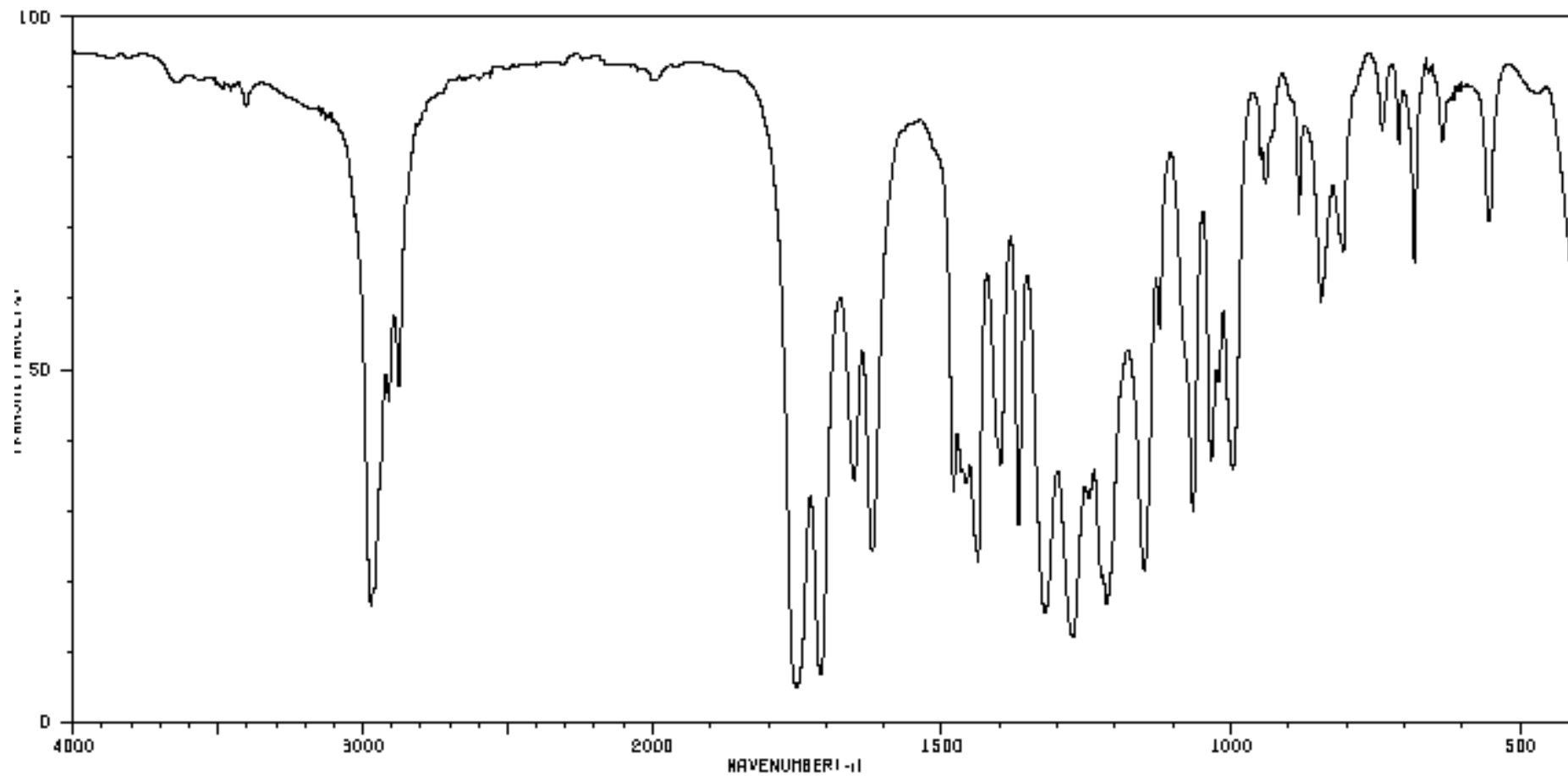


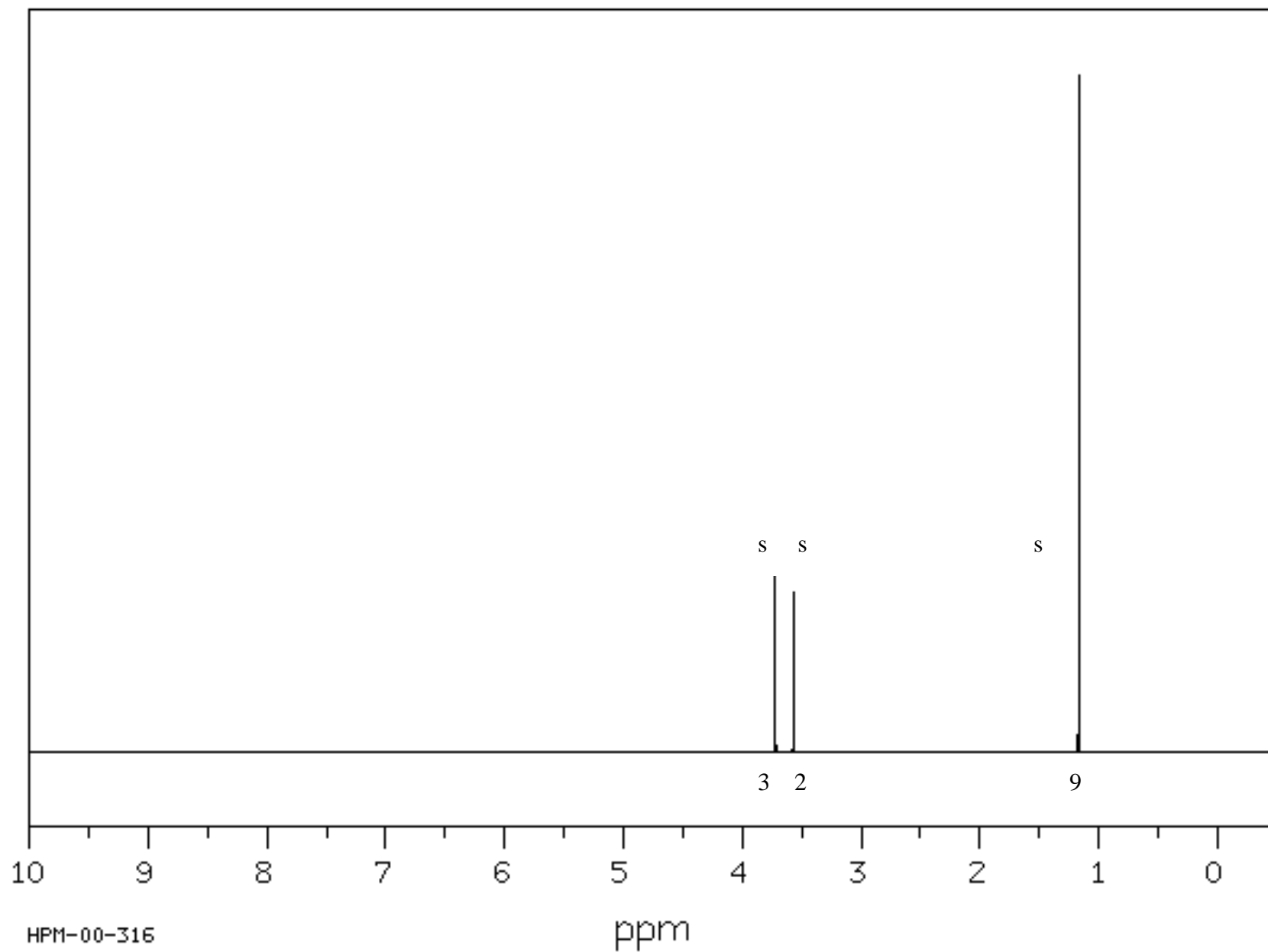


HSP-45-691

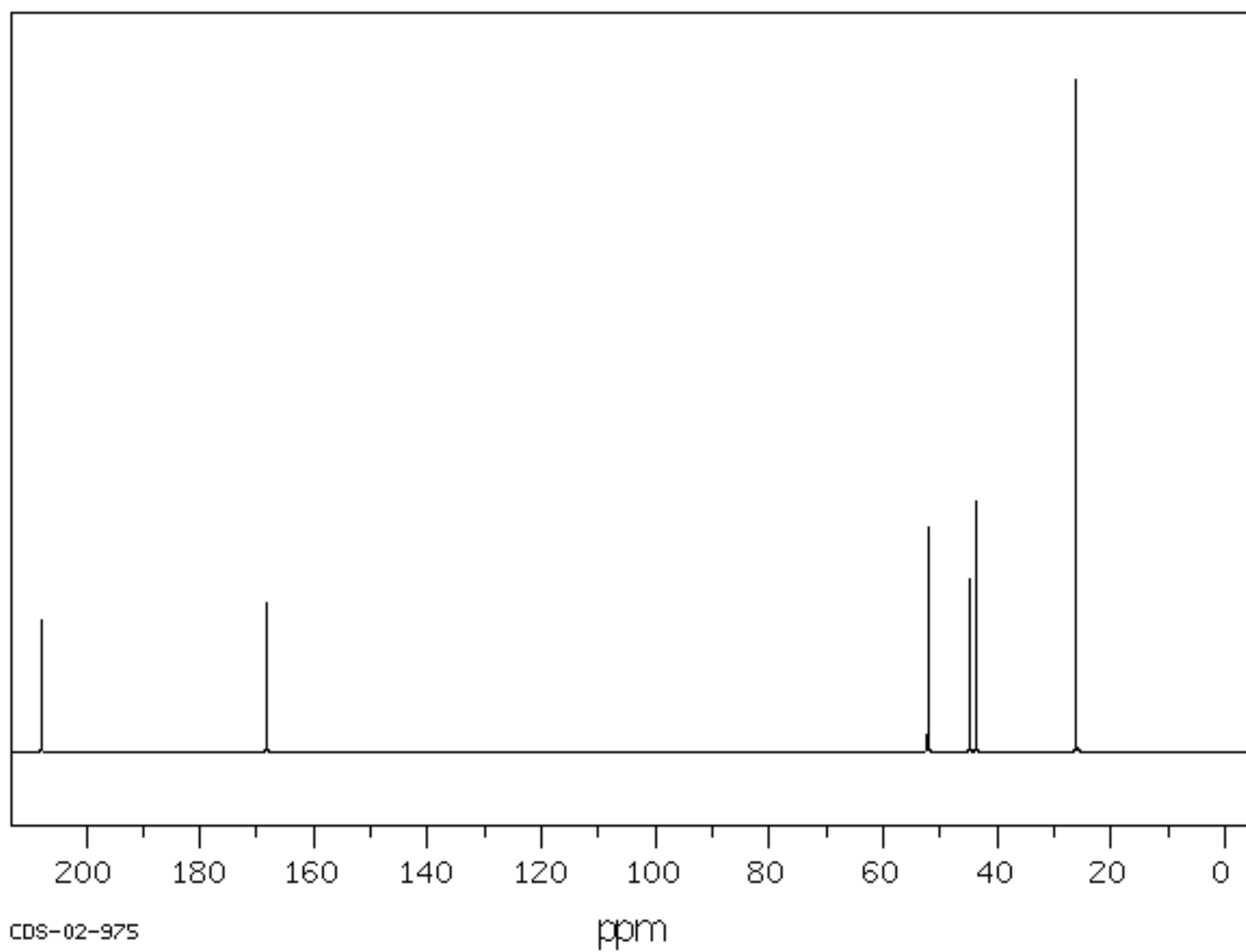


3. $C_8H_{14}O_3$

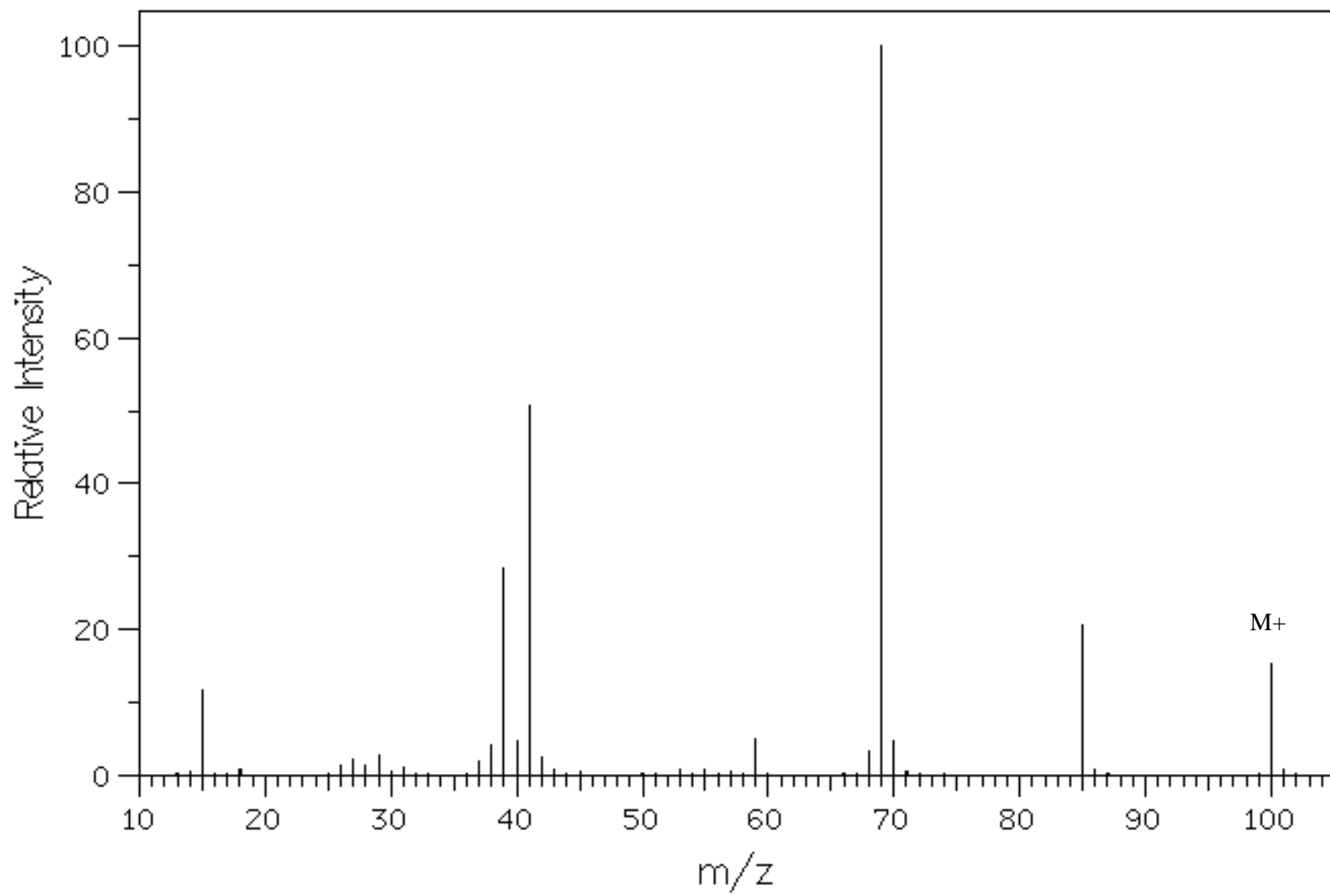


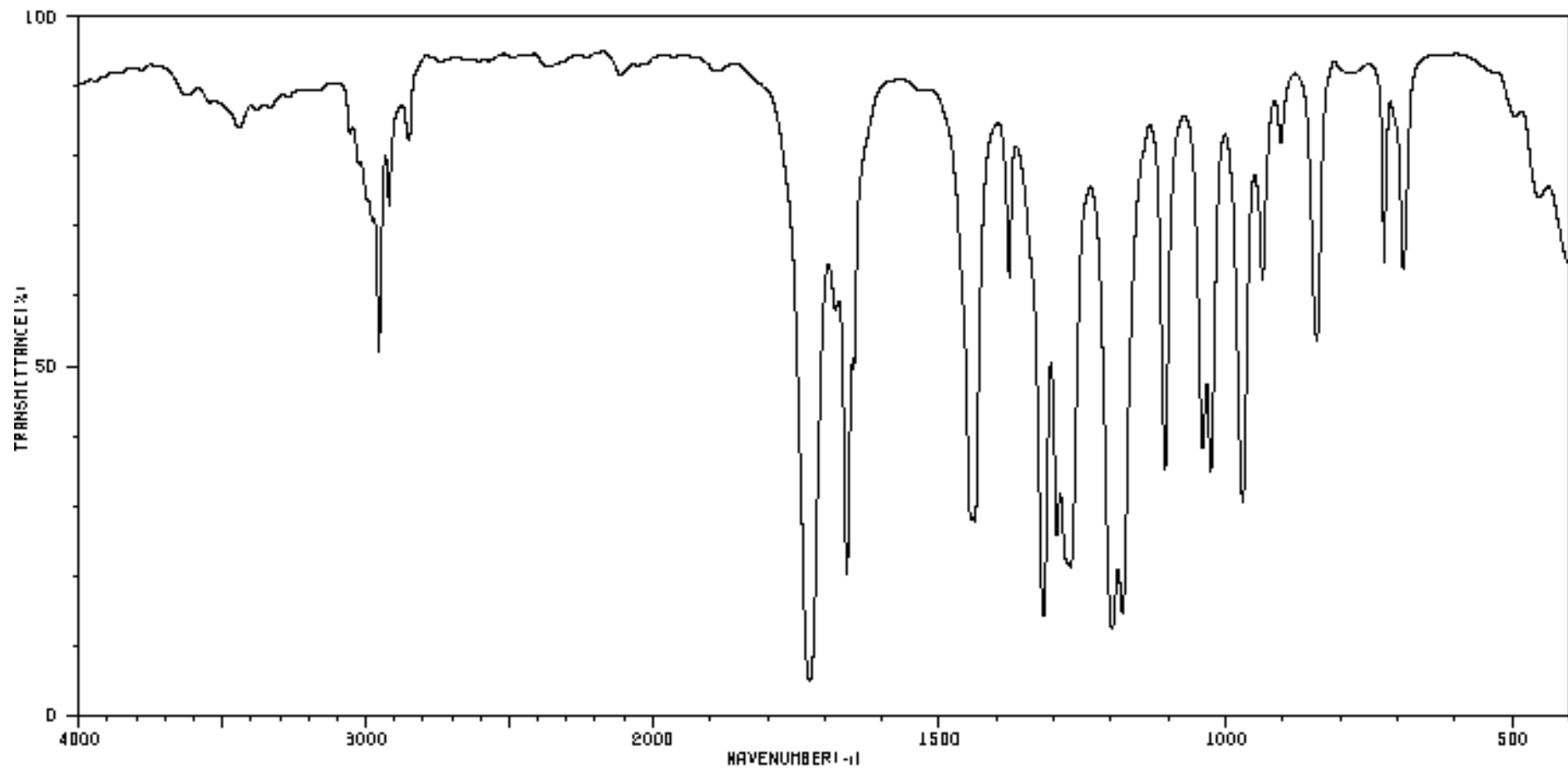


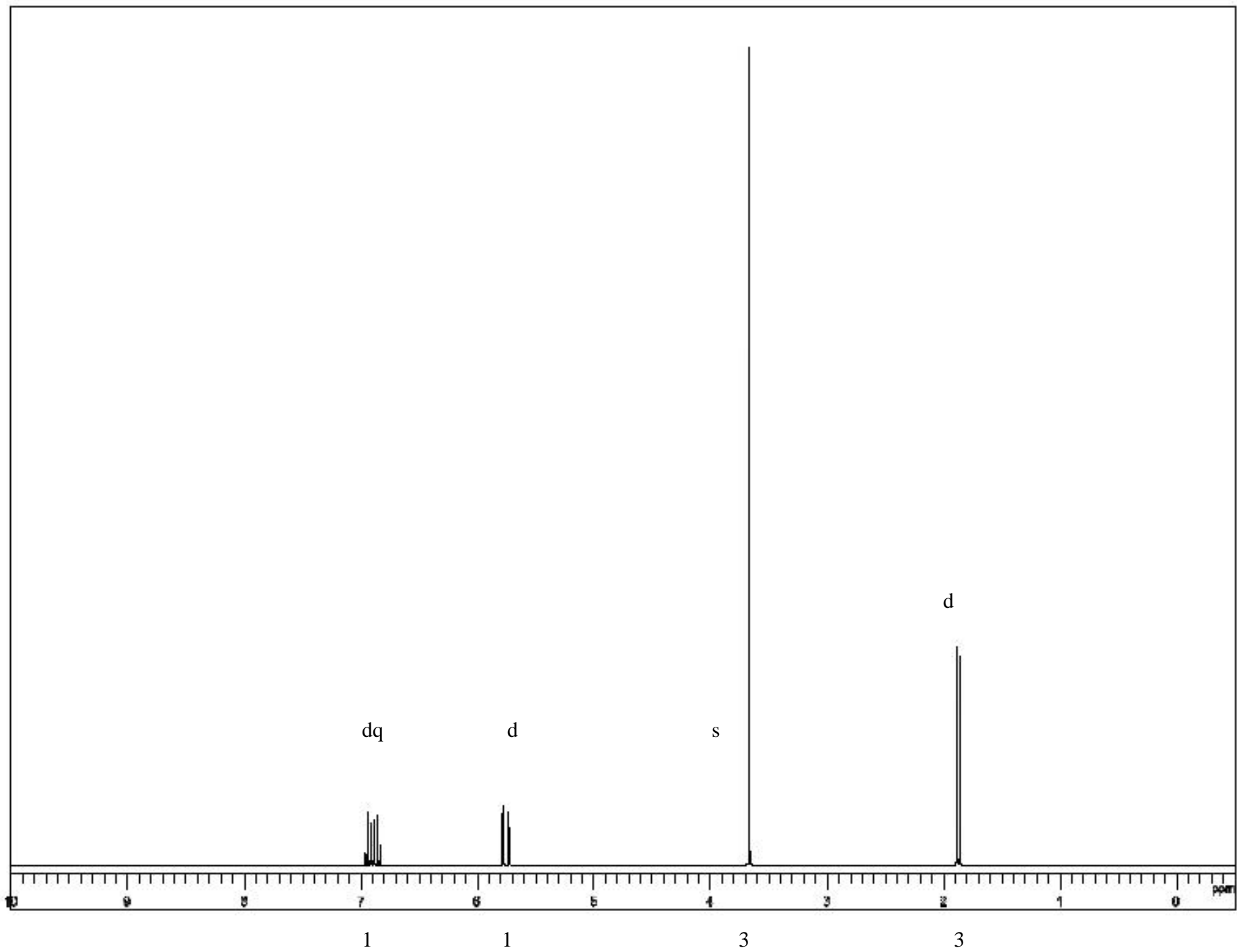
HPM-00-316

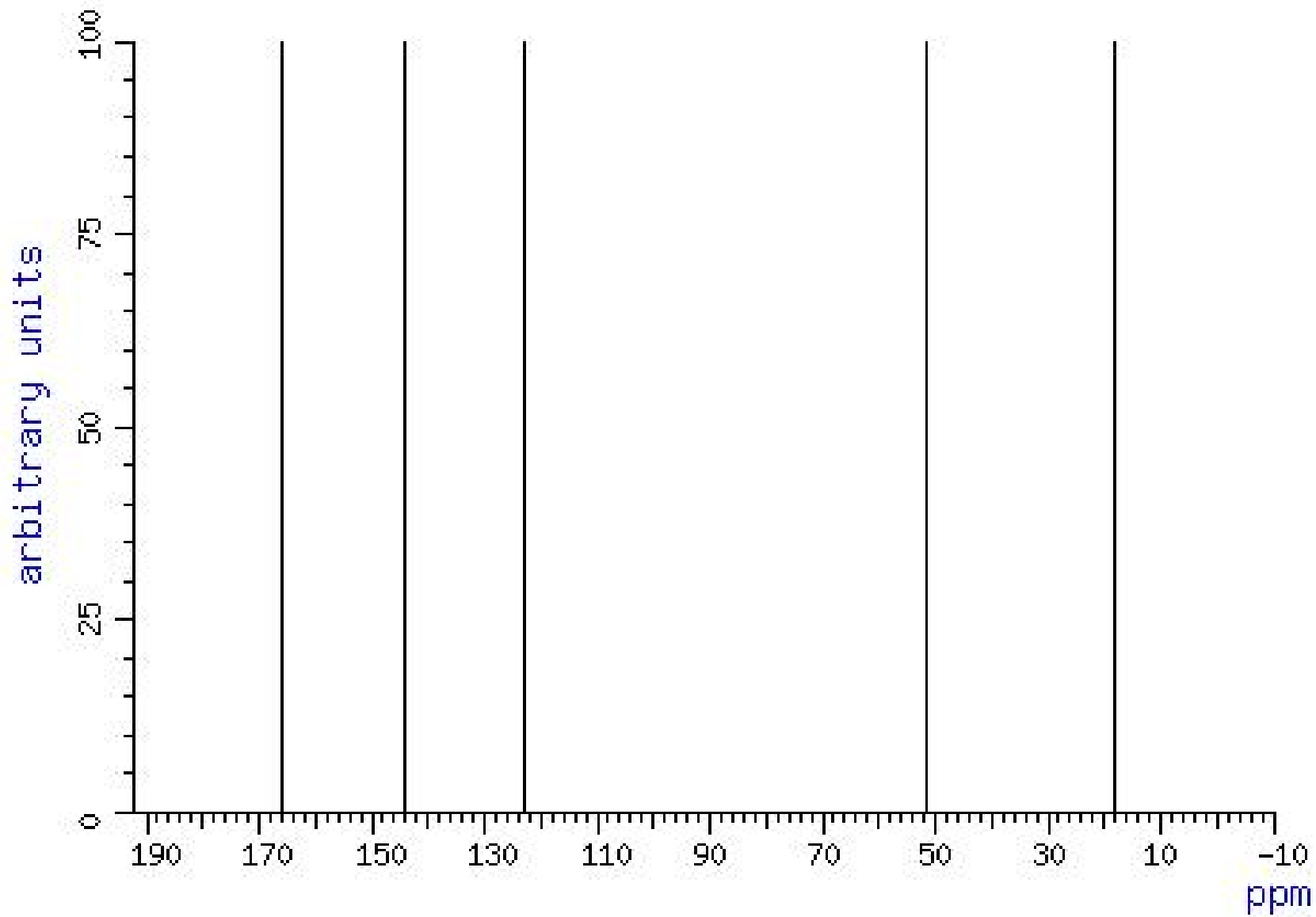


4.

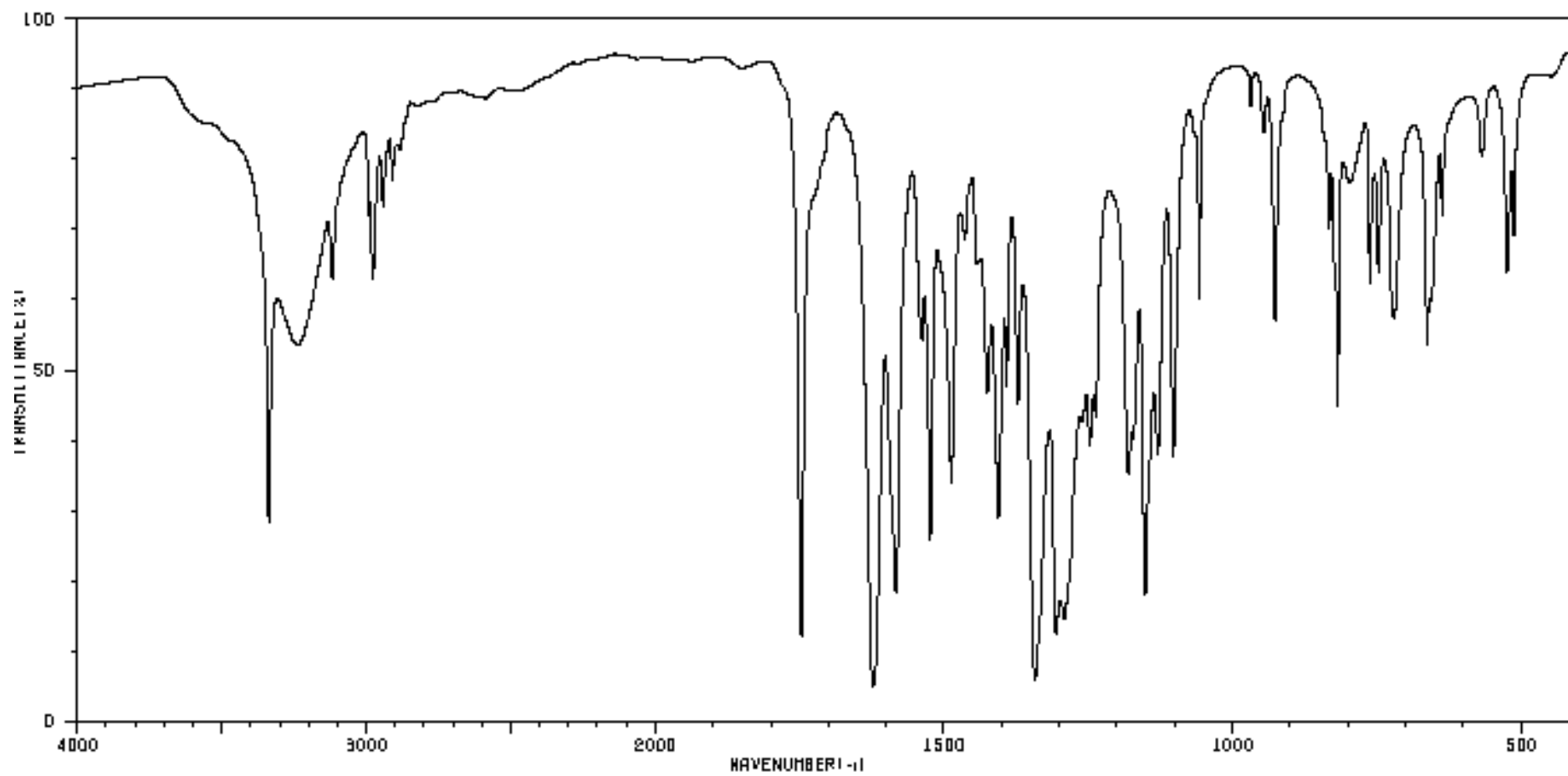


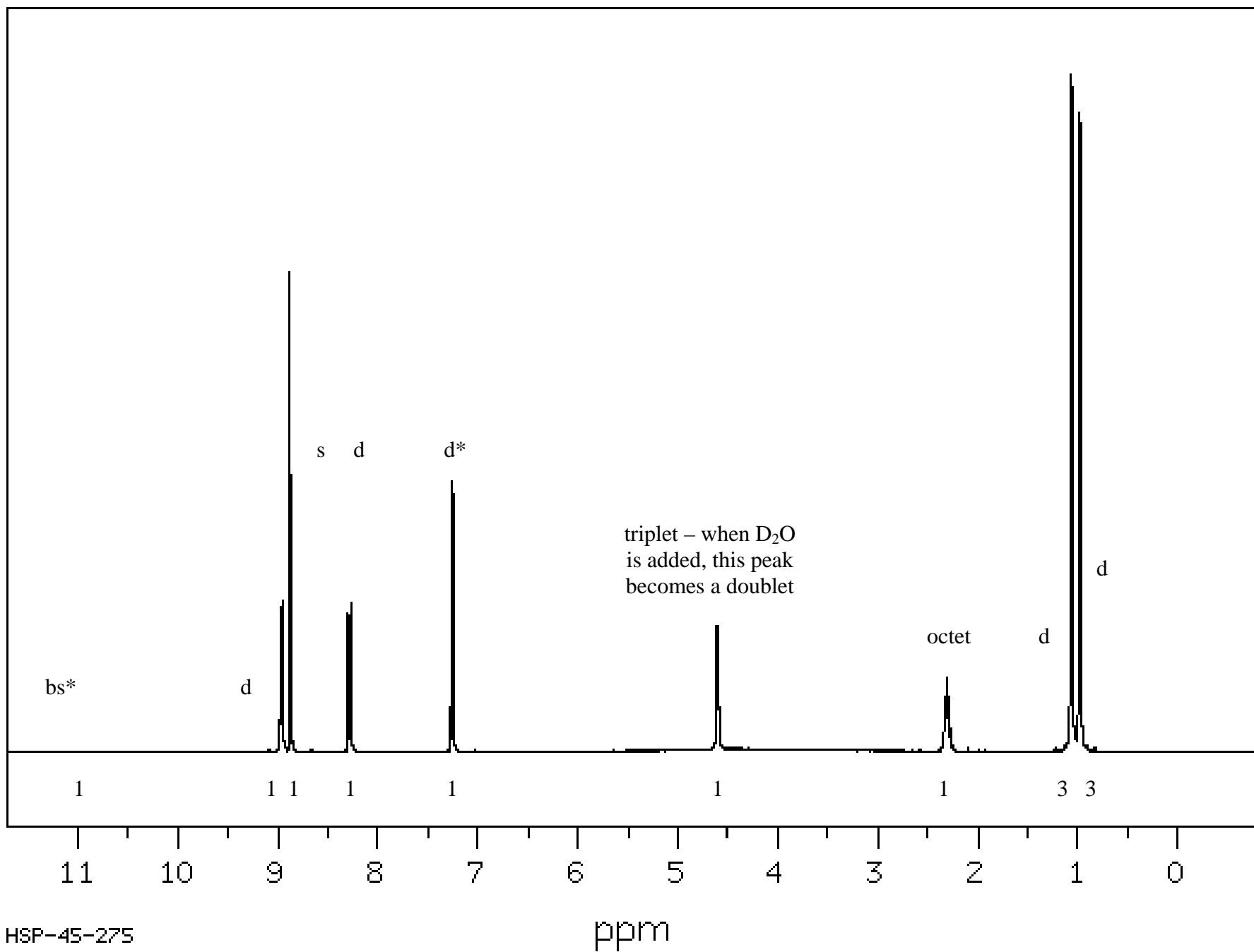




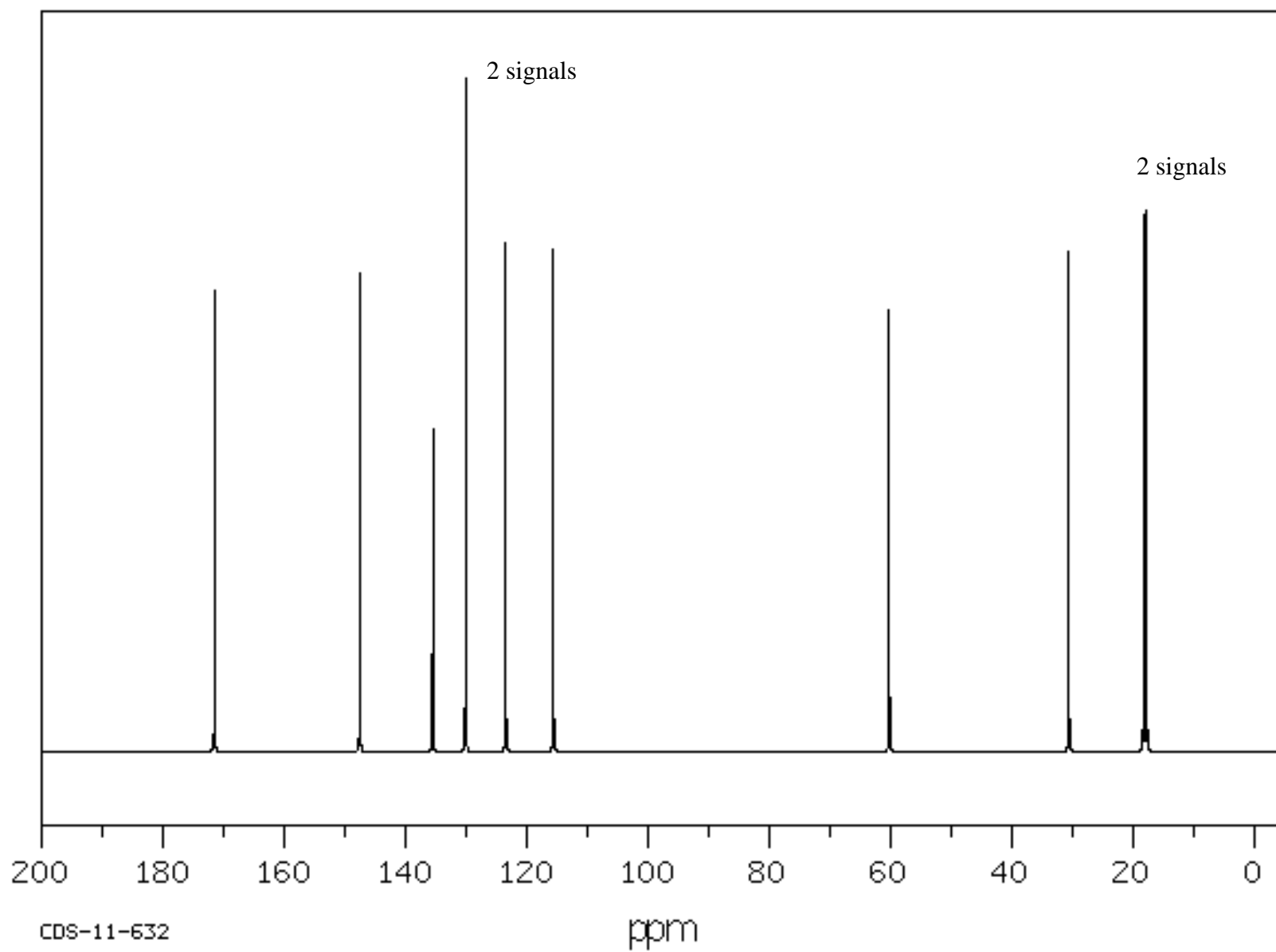


5. $C_{11}H_{13}N_3O_6$





HSP-45-275



6.

(Mass of molecular ion: 182)

