

Proving the Identity of p-bromonitrobenzene by Means of Modern Analytic Techniques

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1 Introduction

This essay serves to prove the identity of para-bromonitrobenzene (see Figure 1) with the use of three different modern analytic techniques – namely: H-NMR spectroscopy, IR spectroscopy and mass spectrometry. To prove the compound's identity, the obtained spectra were analyzed and compared to the expected spectra.

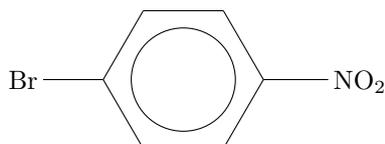


Figure 1: Diagram of para-bromonitrobenzene.

2 H-NMR Spectroscopy

The H-NMR spectrum contained 7 notable peaks which met a certain threshold, as shown below in Table 1.

Index	ppm
1	8.121
2	8.099
3	7.707
4	7.684
5	7.262
6	1.551
7	0.000

Table 1: Table of H-NMR peaks above a certain threshold.

Upon further analysis, however, it is visible that peaks 1 and 2 are most probably not two singlets, but rather just one peak with a higher multiplicity (e.g. a doublet); the same also applies for peaks 3 and 4 – this will be confirmed

later when looking at the spectrum itself. The remaining peaks, with indexes 5, 6 and 7, almost certainly do not correspond to the compound itself, because:

- peak 5 has a ppm value of 7.262, which is characteristic for samples where chloroform is the solvent [1].
- peak 6 has a ppm value of 1.551 which corresponds to water in samples where chloroform is the solvent (Ibid)
- peak 7 has a ppm value of 0.000, which suggests it was used to calibrate the ppm values for all peaks

Peaks 1, 2, 3 and 4 are therefore the only ones which pertain to the compound itself. Figure 2 (see below) shows the portion of the spectrum relevant to these peaks.

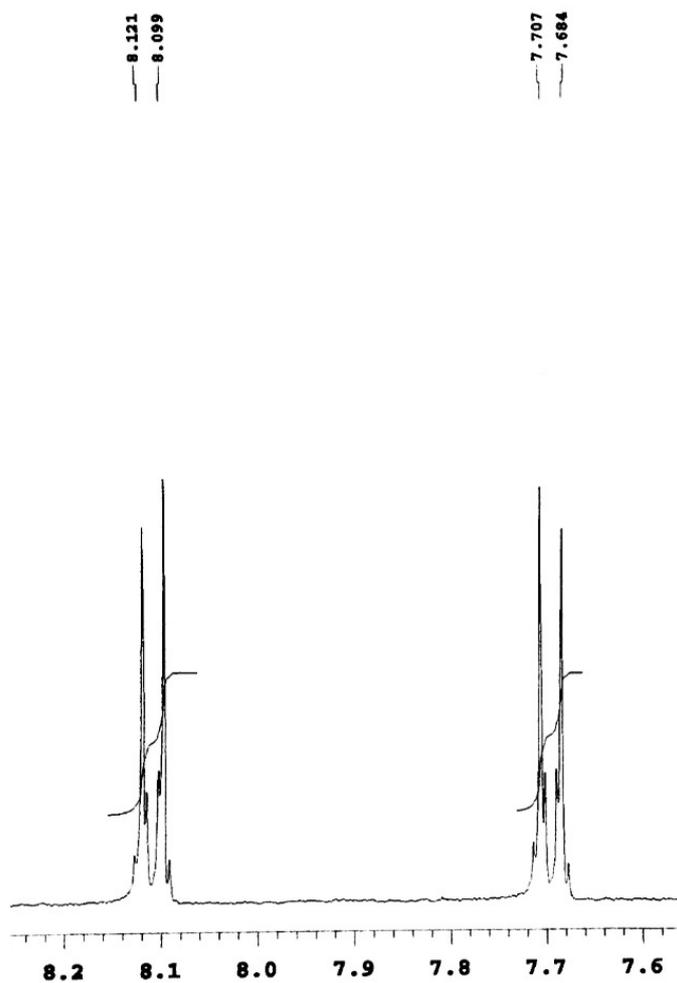


Figure 2: H-NMR spectrum of the substance in the range between 7.6 and 8.2 ppm.

The spectrum confirms the suspicions that the previously-labeled peaks 1 and 2, as well as 3 and 4 are not multiple singlets but rather single peaks with a higher coupling. None of these ppm values are included in the IB Chemistry data booklet, however, they match with the expected values for the supposed compound, according to the Spectral Database for Organic Compounds [2].

3 IR Spectroscopy

The IR spectrum for the received substance (seen below in Figure 3) shows 2 important peaks. A peak at 3000-3100 cm^{-1} , which corresponds to the =C-H structures in alkenes or aromatic compounds, suggests the presence of a benzene ring [3]. A second notable peak occurs at 1520 cm^{-1} which corresponds to the presence of the NO_2 group [4].

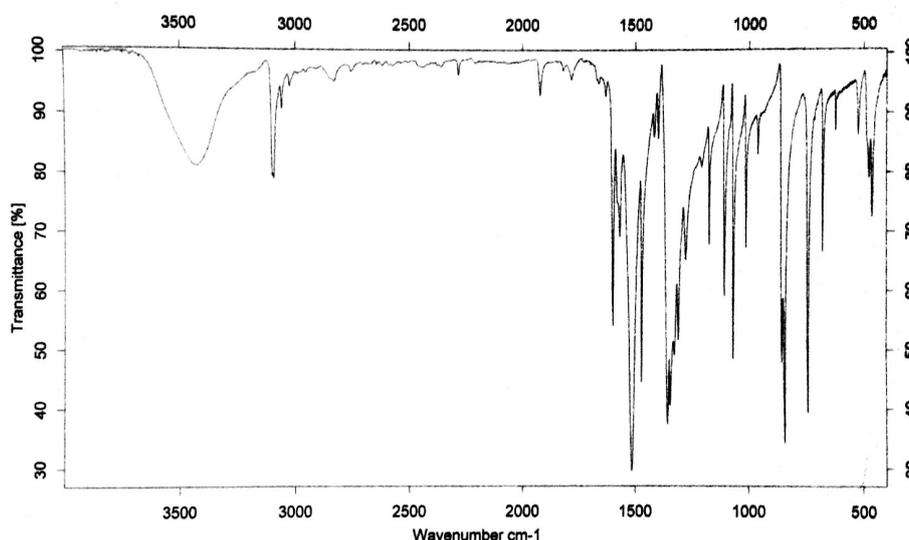


Figure 3: IR spectrum of the substance

4 Mass Spectrometry

The final method of analysis was by mass spectrometry. The spectrum obtained can be seen on the next page, in Figure 4.

What immediately comes to notice when looking at the spectrum is how it is unclear which peak corresponds the molecular ion. This is because bromine has two isomers, Br^{79} and Br^{81} . Knowing this, by averaging the values of the two molecular ion peaks at 201.1 m/z and 203.1 m/z , the mean molar mass of the compound is found to be 202.1 – which is the expected value for p-bromonitrobenzene. The remaining peak data is analyzed in the following table (Table 2), where the peaks containing different isotopes of bromine have been averaged for the purpose of simplicity. The second notable peak (after the molecular ion peak) occurs after a drop of 46 m/z , which matches the

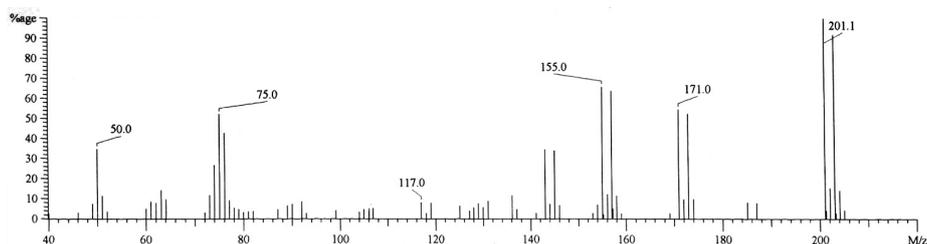


Figure 4: Mass spectrum of the substance.

expected outcome when removing an NO_2 group (as would happen with p-bromonitrobenzene), and then, as expected, the next fragmental ion appears a further 80 m/z below, which corresponds with the average mass of Br. What remains has a m/z value of 76 – very likely from a C_6H_4^+ fragmental ion. The spectrum's main features entirely fit with what would be expected from the proposed substance.

Average m/z	Ion Formula	Average m/z Lost	Group Lost
202	$\text{C}_6\text{H}_4\text{BrNO}_2^+$	N/A	N/A
156	$\text{C}_6\text{H}_4\text{Br}^+$	46	NO_2^+
76	C_6H_4^+	80	Br^+

Table 2: Table briefly and simply analyzing the mass spectrometry peaks.

5 Conclusion

The received substance matches its proposed identity of para-bromonitrobenzene. The spectra are all as would be expected when analyzed, and compare well to the material available online for the compound. If further confirmation of the compound were needed, the physical properties could also be examined as well as its chemical reactions.

References

- [1] C. A. Merlic, *Notes on NMR Solvents*. 2nd edition, 1997.
Spectral Database for Organic Compounds SDBS.
<<http://www.chem.ucla.edu/~webspectra/NotesOnSolvents.html>>
- [2] SDBSWeb, *Spectral Database for Organic Compounds SDBS*.
<<http://sdb.srioddb.aist.go.jp>>
- [3] *IR Spectroscopy Tutorial: Aromatics*.
<<http://orgchem.colorado.edu/Spectroscopy/irtutor/aromaticsir.html>>
- [4] *Infrared spectroscopy correlation table*. Wikipedia.
<http://en.wikipedia.org/wiki/Infrared_spectroscopy_correlation_table>