Portfolio of Original Compositions

A thesis submitted to the University of Manchester
for the degree of Doctor of Philosophy
in the Faculty of Humanities

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Falk Morawitz

School of Arts, Languages and Cultures
Contents

List of tables 6
List of figures 6
Portfolio of musical work 9
USB content 10
Abstract 12
Declaration 13
Copyright statement 13
Technical information 14
About the author 16
Acknowledgement 16

Written commentary

1 Introduction 18
   1.1 Portfolio contents 18
   1.2 Research enquiry 18
   1.3 Chapter outline 19
   1.4 Nomenclature and form 19

2 Background 20
   2.1 An Introduction to sonification 20
   2.2 Chemical data and sonification 21
   2.3 An introduction to spectroscopy 22
      2.3.1 Spectroscopic sonification in scientific research 24
      2.3.2 Spectroscopic sonification in music composition 24
3 Spin Dynamics

3.1 Data sources and sonification methodology

3.1.1 An Introduction to nuclear magnetic resonance spectroscopy

3.1.2 1H-NMR and 13C-NMR sonification methodology

3.1.3 Characterisation of obtained sound morphologies

3.2 Structure

4 Inner Resonance

4.1 Data sources and sonification methodology

4.1.1 Solid state nuclear magnetic resonance spectroscopy

4.1.2 Sonification of hydrogen-1 solid-state NMR data

4.2 The bass clarinet and sonification

4.3 Structure

5 Quantum

5.1 Data sources and sonification methodology

5.2 Spectroscopic sonification in virtual reality

5.2.1 Setup and controls

5.2.2 Thoughts on interactive sonification in virtual reality

5.3 Structure

6 Darkest Hour

6.1 Data sources and sonification methodology

6.2 Additional sound sources

6.3 Tonal progressions

6.4 Sonification and moving images
7  Finland, as experienced by the Sea  
7.1  Data sources and sonification methodology  
7.1.1  Pollution problems in the Baltic Sea  
7.1.2  Data sources  
7.1.3  Structure  
7.2  Presentation  
8  On the Extinction of a Species  
8.1  Data sources and sonification methodology  
8.2  Additional sound sources  
8.3  Structure  
8.4  Acousmatic storytelling and sonification  
9  56Fe  
9.1  Data sources and sonification methodology  
9.1.1  Water orbital data sonification  
9.1.2  Iron orbital data sonification  
9.1.3  Sound characteristics and sonification procedure  
9.2  Structure  
10  Conclusion  
10.1  Aesthetic implications and sound affordances  
10.2  'Paramedia' and modes of information communication  
10.3  The incorporation of extra-musical ideas via data sonification  
10.4  Addressing research questions  
10.5  Research contributions  
10.6  Future work
10.6.1 Unexplored spectroscopic data types 70
10.6.2 Modes of presentation 71
10.6.3 Voice and storytelling 71

11 Bibliography 72

Appendices 78
A Glossary 78
B Publications 80
C List of performances and presentations 92
D Inner Resonance music score 95
E Introduction to NMR analysis 103
F NMR sonification coding 104
G Sonification of infra-red spectroscopy data 106
H Setup and technical requirements for Quantum 108
I List of video and sound sources for Darkest Hour 110
J Pollution trends in the Baltic, 1940 – 2010 113
K The oceanographic sonification interface and its modules 115
L Structure of On the Extinction of a Species (high resolution) 121
M On the Extinction of a Species transcript 122
N Portfolio program notes 124

Word count: 15000
List of tables

1. Comparison of NMR spectra of different nuclei.
2. Music parameter mapping of section B. Notation after Hermann.
3. Parameter mapping for section C.
4. Parameter mapping for section D.
5. Parameter mapping for section E.
6. Parameter mapping for section F. Plastic concentration measured in percent of fish found with quantifiable ingested plastic residues. Data by Rummel et al.

List of figures

1. Loudspeaker arrangement and assignment for Spin Dynamics. Arrow indicating listening direction.
3. Sonification scheme for the transformation of NMR data to sound, as described by Morawitz.
4. A solid-state 1H-NMR signal depicting one signal and corresponding sidebands.
5. Sonification scheme for solid-state NMR data.
6. Overtone series on A2. In this series, adjacent notes are always 110 Hz apart.
7. Quantum, screenshot.
8. Setup, including VR headset, a leap motion tracker, a standard Xbox controller and various screens displaying the virtual environment.
9. The ringing frequencies of propanol measured using a 500 MHz spectrometer. Frequency data assigned to their nuclei of origin.
Ratio of starting material and product (X) over time, simulated for different initial conditions using the Györgyi-Field Model and code developed by Binous et al.

The Belousov-Zhabotinski line drawings as seen in *Darkest Hour*.

Overlay of Belousov-Zhabotinski lines with footage of marching soldiers.

A Max/MSP algorithm analyses 1 pixel-wide cross sections of an idealized Belousov-Zhabotinski reaction and expands the cross sections to black and white line drawings.

Belousov-Zhabotinski lines as part of the visual transformation. The words seen on screen are derived from material stored in the PHM archives.

Screenshot of a section of the custom-made sonification sequencer, displaying a data display window in the upper half of the screen and two sound modules in the lower half.

Normalized concentration changes for DDT/PCB, nitrate and phosphate, caesium-137 and plastic pollutants in the Baltic Sea. Data sources referenced in chapter 7.2.

Translation of pollution trends to a compositional structure. Every year of pollution data is compressed to ten seconds of composition.

General structure of PCB.

Structure of DDT.

Infra-red spectrum of DDT.

General overview of sound type distribution.

56Fe was premiered as sound installation. Participants were asked to enter a small darkened enclosure. Loudspeakers were hidden within the folds of the textile walls in proximity to the listener, creating a sense of immediacy and intimacy.
Orbitals of oxygen (red) and hydrogen (blue) re-combine when forming H2O, leading to new hybrid orbitals (green). Orbital energy in electron volt (eV), computed by Ning et al.

Ionisation spectrum of water measured at an impact energy level of 1200 eV, computed by Ning et al.

When two or more atoms bond, their orbitals will form new, mixed orbitals above and below the energy level of the original orbitals. If enough atoms bond together, the gap in energy level between these orbitals becomes negligible and energy bands are formed.

Energy distribution of electrons in metallic iron, data from Dronskowski.

Spectrograms of sonifications of iron electron energy level data for various bandpass filter widths.

Periodic system of the elements displaying all elements with NMR-active nuclei.
Portfolio of musical works

1. *Spin Dynamics* 2016 8-channel fixed media 9'50
2. *Darkest Hour* 2016 Stereo fixed media and video 11’28
3. *Inner Resonance* 2016 Bass-clarinet and live electronics 6’03
4. *Quantum* 2017 Virtual reality installation, binaural, open form ±15’00
5. *Finland, as experienced by the Sea* 2017 Stereo fixed media 8’04
6. *On the Extinction of a Species* 2018 7.1-channel fixed media 20’58
7. *56Fe* 2018 Stereo fixed media 9’00

Total duration: 80’30
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All .wav files rendered at 24-bit, 48 kHz.

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<td>Eight sound references for <em>Inner Resonance</em>, labelled as described in Appendix D.</td>
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Abstract

Sonification is broadly defined as the display of data as sound, and has been used in educational, scientific and industrial settings to explore, find and monitor patterns and changes in data. Sonification has also played a vital role in music composition as a technique that offers new methodologies for the creation and structuring of sound, and for the representation of non-musical matters in music. Although numerous examples of artistic sonification exist, the use of spectroscopic data in music composition has not yet been assessed systematically.

Spectroscopic analysis is concerned with the interaction of electromagnetic radiation and physical matter. The portfolio explores the use of spectroscopic data in electroacoustic composition to find new methodologies for creating and structuring sound. It examines the role of spectroscopic data in acousmatic, audio-visual, and virtual reality works and investigates how electroacoustic compositions using spectroscopic data can be used to raise awareness of current environmental and socio-political challenges.

The portfolio comprises seven electroacoustic works. Spin Dynamics is an acousmatic music composition that uses nuclear magnetic resonance (abbr. NMR) data as its only sound source. Inner Resonance explores the interplay between solid-state NMR sonification and the bass clarinet. Quantum combines NMR data with visual stimuli in an interactive virtual reality environment. The refugee crisis is contextualised in the audio-visual work Darkest Hour. Finland, as experienced by the Sea, presents pollution trends in the Baltic Sea using a mix of NMR, infra-red, and oceanographic data sonification. On the Extinction of a Species explores the sonification of DNA sequences of an extinct species to raise awareness of humanity's reckless treatment of its environment. Sound pollution and our relationship with technology are traced in $56Fe$ using the sonification of electron energy level data.

The portfolio and written commentary contribute to the field of electroacoustic composition by presenting and evaluating methodologies for the sonification, framing, and presentation of spectroscopic data. Promising avenues of future work are discussed.
Declaration

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**Technical information**

All sound material is presented in 48 kHz, 24-bit resolution.

**Works with live electronics (Inner Resonance)**

The setup and technical requirements for *Inner Resonance* are included in the score which can be found in Appendix C. The Max/MSP patch can be found on the USB flash drive under \*:\2Supplementary\CodingAndSoftware\InnerResonanceLivePatch

**Multi-channel works**

Speaker arrangements for multi-channel pieces can be found below. Stereo versions of multi-channel pieces are provided for reference purposes.

**8-channel (Spin Dynamics)**

The piece *Spin Dynamics* is submitted as eight labelled mono files. Each mono file is numbered from 1 to 8 and is to be assigned the correct speaker according to figure 1 below.

**Figure 1**: Loudspeaker arrangement and assignment for *Spin Dynamics*. Arrow indicates listening direction.
7.1-channel (On the Extinction of a Species)

The piece *On the Extinction of a Species* is submitted as eight mono files. Each mono file is labelled and is to be assigned the correct speaker according to figure 2. Please note that the piece does not follow a regular 7.1 speaker arrangement pattern but consists of a 5.1 channel arrangement (L, C, R, Ls, Rs) and additional stereo pair (1, 2), the latter designed for live diffusion.

![Figure 2: Loudspeaker arrangement and assignment for On the Extinction of a Species. Arrow indicates listening direction. Grey speakers for live diffusion.](image)

**Audio-visual work**

All audio-visual works and video documentation are rendered using the H.264 video compression codec and will play back using any conventional video playback device.

**Virtual reality installations (Quantum)**

The setup and technical requirements for *Quantum* are detailed in Appendix H.
About the author

The author has a Master’s degree in music composition (University of Manchester, MMus, 2015) and a Master’s degree in chemistry with medicinal chemistry (University of St Andrews, MChem, 2012).

Acknowledgement

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I would also like to thank the NOVARS technicians and postgraduate research community for many fruitful discussions.

I sincerely thank Crystal Kwan Chan for her endless patience, help and support.
Daß ich erkenne, was die Welt
Im Innersten zusammenhält.

Johann Wolfgang von Goethe - Faust
1. Introduction

Sonification is the transformation of data into sound and has been used by scientists and artists for the exploration, communication, and presentation of data. Composers have utilized sonification as a tool to create and arrange sound materials. This portfolio of works adds to the field of sonification by systematically exploring the use of spectroscopic data sonification (the sonification of energy absorption and emission patterns of atoms and molecules) in electroacoustic music composition.*

1.1 Portfolio contents

This portfolio of compositions contains seven electroacoustic compositions in the form of one stereo and two multi-channel fixed media pieces, one mixed media work, one audio-visual piece, one virtual reality audio-visual environment, and one sound installation.

1.2 Research enquiry

This practice-based portfolio contributes to the field of sonification and electroacoustic composition by addressing the following research questions:

1. How can the sonification of spectroscopic data act as a creative vehicle and innovator for contemporary electroacoustic compositional practices?

2. How do the format, presentation, and paramedia* of a composition using spectroscopic sonification influence the work’s reception and the listener’s aesthetic experience?

3. In what way can socio-cultural connotations towards science be used in sonification-based musical compositions and sound art installations to raise awareness of major environmental and socio-political challenges?

* A further introduction to sonification and chemical spectroscopy can be found in Chapter 2 - Background.

* In this context, paramedia refers to all material surrounding a creative work that is not part of the work itself, for example program notes or a lecture about the work. Paramedia is a newly proposed term, in definition similar to paratext, the latter describing all written works supporting a main literary text. Please see appendix A for a further discussion of the term.

1.3 Chapter outline

Chapter 2 sets out the key terms and definitions in the field of sonification followed by an illustration of the history and use of spectroscopic sonification in science and art. Chapter 3 presents the compositional process of Spin Dynamics, an acousmatic music composition that uses nuclear magnetic resonance (abbr. NMR) data as its sound source. Inner Resonance, described in chapter 4, explores the interplay between solid-state NMR sonification and the bass clarinet. Chapter 5 explains the thought process behind Quantum, an installation piece combining NMR sonification with visual stimuli in a virtual reality environment.

The second part of the written commentary disseminates portfolio works contextualising environmental and socio-political issues. Chapter 6 describes Darkest Hour, an audio-visual work in which audio and visual components were transformed by chemical reaction dynamics. Chapter 7 describes Finland, as experienced by the Sea, an acousmatic composition based on nuclear magnetic resonance, infra-red and oceanographic data sonification of pollutants in the Baltic Sea. Chapter 8 contextualises On the Extinction of a Species, exploring DNA sequence sonification of the passenger pigeon, an extinct species, to raise awareness of humanity’s reckless treatment of its surroundings. Chapter 9 describes 56Fe, a sound installation on sound pollution and our relationship with technology, based on the sonification of electron energy levels. The commentary closes with a summary and conclusions, detailing key findings and possible future avenues of research.

1.4 Nomenclature and form

The portfolio makes use of the terminology developed by Smalley\(^2\,^3\) for the description of the spectromorphological and spatiomorphological qualities of sound. Titles of artistic and musical works appear in italics throughout the document. A glossary on key terms of sonification and spectroscopy can be found in Appendix A.


\(^3\) Denis Smalley, "Space-Form And The Acousmatic Image", Organised Sound, 12.01 (2007), 35.
2. Background

2.1 An introduction to sonification

“Sonification is defined as the use of non-speech audio to convey information. More specifically, sonification is the transformation of data relations into perceived relations in an acoustic signal for the purposes of facilitating communication or interpretation.” - Kramer et al.4

Sonification is an interdisciplinary field concerned with the transformation of data into sound and has been explored in a wide variety of disciplines such as the natural sciences, mathematics, psychoacoustics, psychology, human-computer interactions, and music composition.5 Sonification has proven to be of considerable use particularly in finding trends,6 patterns,7 or small fluctuations8 in data, due to our highly developed auditory cognition and our ability to analyse sound morphologies and sonic gestalt features. Sonification has been successfully employed for the exploration of scientific datasets9 and the monitoring of biological and industrial processes.10

As sonification offers an opportunity to listen to a world that is normally hidden from our senses, it has been incorporated into music compositions and sound art. As a creative methodology, sonification offers the opportunity to make abstract data perceivable.11,12 It offers new methodologies for creating and structuring sound,13 and for representing non-musical concepts in music compositions.14 Intriguingly, music compositions based on

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9 Ibid.
scientific data or mathematical models have been reported to be perceived as 'science and not art'\textsuperscript{15} that 'in various ways [claim] a sort of objectivity'.\textsuperscript{16} It is argued that the attribution of scientific qualities to an artistic work can change the aesthetic experience and the way the work is interpreted by the listener,\textsuperscript{17,18} adding another layer of content and context for artists to explore and incorporate.

2.2 Chemical data and sonification

The use of chemical data has been explored in educational contexts, for example in the creation of data analysis tools for the visually-impaired\textsuperscript{19,20} or molecular displays in virtual reality.\textsuperscript{21} In scientific research, sonification has been used to find reoccurring patterns and structural features in big datasets, most notably for pattern recognition of DNA sequences,\textsuperscript{22} and for assessing structural features in large macro-molecules.\textsuperscript{23} Chemical data have been used as a tool to explore new facets of sound creation and structuring in music composition as well as for the encapsulation of extra-musical ideas. One example of the latter is Mario Duarte’s piece \textit{Ayotzinapa} commemorating the death of 43 Mexican students by targeted police killings by encoding their names as DNA codons for subsequent sonification.\textsuperscript{24}

A wide variety of chemical data types have been explored in music composition including data on dynamic molecular systems,\textsuperscript{25} Brownian movement,\textsuperscript{26} protein folding energy data,\textsuperscript{27}

\begin{thebibliography}{99}
\bibitem{18} David Glowacki, "Using Human Energy Shields to Sculpt Real Time Molecular Dynamics", \textit{Molecular Aesthetics}, 1, (2013), 4, pp. 246 – 257; here, 249.
\bibitem{19} David Lunney, "Development Of A Data Acquisition And Data Analysis System For Visually Impaired Chemistry Students", \textit{Journal Of Chemical Education}, 71.4 (1994), 308.
\bibitem{21} Christine M. Byrne, "Water On Tap The Use Of Virtual Reality As An Educational Tool" (Ph.D. Thesis, University of Washington, 1996).
\bibitem{26} E.g. Iannis Xenakis, \textit{PH Concrete}, 1958.
\end{thebibliography}
or DNA base pair sequences.\textsuperscript{28,29} There is surprisingly little documentation on the artistic use of spectroscopic data, a datatype which, as will be elaborated in the following chapters, offers a variety of unique features for sonification in an electroacoustic context.

2.3 An introduction to spectroscopy

Spectroscopic studies are standard procedures in chemistry that use electromagnetic radiation to investigate the structure and other properties of chemical compounds.\textsuperscript{30} Every part of the electromagnetic spectrum interacts with a different state of a chemical compound. A variety of spectroscopic methods have been derived and refined to make use of these interactions to gain insights into the structure, bonding strength, geometry and other aspects of chemical compounds (Table 1). Almost every type of chemical interacts differently with the electromagnetic spectrum, resulting in different spectra for each. The sonification of spectroscopic data therefore promises to create a wide range of compound-specific timbres. Spectra of millions of chemical compounds can be found online\textsuperscript{28-33} but even though spectroscopic data are freely available and its sonification can give rise to a wide array of timbres, most spectroscopic data have received little consideration as a sound source for the creation of electroacoustic music compositions.

\textsuperscript{29} Mario Duarte Garcia, "Portfolio of Original Compositions" (Ph.D. Thesis, University of Manchester, 2018).
\textsuperscript{32} "Nmrshiftdb2 - Open Nmr Database On The Web", \textit{nmrshiftdb.nmr.uni-koeln.de}, <http://nmrshiftdb.nmr.uni-koeln.de/> [Accessed 31 July 2018].
\textsuperscript{34} "1H-NMR database",http://www.chem.wisc.edu/areas/reich/handouts/nmr-h/hdata.htm [Accessed 03 January 2016].
\textsuperscript{35} "Nmrshiftdb2 - Open Nmr Database On The Web", \textit{nmrshiftdb.nmr.uni-koeln.de}, <http://nmrshiftdb.nmr.uni-koeln.de/nmrshiftdb/media-type/html/user/anon/page/default.psml/js_pane/P-Search> [Accessed 03 January 2016].
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<td><img src="image.png" alt="Diagram" /></td>
<td><img src="image.png" alt="Diagram" /></td>
</tr>
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<table>
<thead>
<tr>
<th>Spectroscopic method gives insight into</th>
<th>Molecular structure, presence of functional groups</th>
<th>Molecular structure in gas phase, gas interactions</th>
<th>Bond strengths, structure, functional groups</th>
<th>Electron configuration and electron energy</th>
<th>Atomic shell energy levels</th>
</tr>
</thead>
</table>

Table 1: An overview of spectroscopic methods used in analytical chemistry.
2.3.1 Spectroscopic sonification in scientific research

Spectroscopic sonification has been used to find data fluctuations that are too small to detect by visual inspection alone and are hard to distinguish from the random fluctuations of the noise floor, for example in finding oscillation coupling between weakly coupled quantum states.\(^{37}\)

In the early 70s, nuclear magnetic resonance spectrometers had optional sound modules that would audify signals in real-time.\(^{38}\) The audio feedback told analysts whether their machine was calibrated correctly and gave an indication of the quality and properties of the resulting spectra.\(^{39}\) For the most part, these sound-producing modules were seen as an oddity, novel enough to program a rendition of 'Happy Birthday'\(^{40}\) but too monotonous and unengaging for daily analytical use. This led to a gradual decline and the eventual end of NMR sonification in the mid-70s.

2.3.2 Spectroscopic sonification in music composition

Spectroscopic sonification has seen sparse engagement from composers. Alexjander et al.\(^{41}\) used prominent peaks in the infra-red (abbr. IR) vibration spectra of DNA bases as microtonal tunings for an instrumental composition. Delatour explored the use of IR peak data for the creation of new timbres by transposing IR absorption frequency data into the audible range.\(^{42},43\) His investigations are based on inverse Fourier transformations of infra-red data and the use of additive re-synthesis for sound creation. He also experimented with mapping IR data to acoustic pressure, pitch, and filter cut-off frequencies during the synthesis process to create a wider variety of sounds based on IR data. Although he

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\(^{39}\) Ibid.


described a methodology for converting IR data into sound, he did not arrange these sounds to form music compositions.

Besides the use of IR data, the use of spectroscopic data has been limited. Many other types of spectroscopic data, including nuclear magnetic resonance data, have not previously been used in electroacoustic composition, but are explored in this portfolio and documented in the following chapters.

2.4 The role of the composer

The creation of a data-driven music composition is a balancing act between scientific authenticity and artistic expression. Whether a music composition puts greater emphasis on the transparent auditory display of data or the exploration of aesthetic affordances of sonified data morphologies depends on a variety of factors, including the purpose of the piece, the morphology of the data, the composer’s background, and the target audience, to name a few.

2.4.1 Sound creation and arrangement methodologies

The portfolio submitted is firmly situated within the realm of electroacoustic music composition. The compositional methodologies developed and employed put a distinct emphasis on the exploration and presentation of aesthetic properties of the sonified data while aiming to preserve a traceable link between sound and data morphologies. This negotiation between scientific and artistic emphasis permeated the compositional process, including data selection, the choice of data sonification techniques, employed sound transformations and sound arrangement choices. Broader compositional decisions are briefly detailed below, whereas piece-specific compositional processes are described in more detail in chapters 3 to 9, respectively.

Most portfolio pieces are based on the sonification of nuclear magnetic resonance data, effectively data of electromagnetic waves with frequencies of up to 20 kHz and attenuation times of up to 30 seconds. This wave data can be sonified in a variety of ways, including audification, re-synthesis of peak data via additive synthesis, FM synthesis and AM synthesis, model-based sonification or spectral convolution, to name a few.

In this portfolio, only audification and additive re-synthesis were employed to create sounds, as these sonification methods involved the least mapping decisions. Audification involved no mapping decisions, whereas, in additive re-synthesis, the phase and attenuation
envelope of each sine wave could be controlled. In both cases, the timbre of the sonified sound is a transparent representation of peak patterns in the nuclear magnetic resonance data. Molecular features, such as the presence of specific functional groups or atomic coupling can be heard in the sonification’s timbre. The attenuation envelope of the NMR data only carries relatively little information in comparison and was altered more readily, according to compositional needs.

2.4.2 A note on background noise in experimental data

The main difference between the audification of experimental data and additive re-synthesis of analysed peak data is that audified experimental FID data contains a noise background that is absent in sounds created via additive synthesis. Noise can often contain additional information and the noise background of FID data can give indications of impurities in the chemical sample. For example, small broad additional peaks in a spectrum can be attributed to the presence of residual solvents from previous chemical reactions. The signal-to-noise ratio in an NMR spectrum is not a straight-forward measure of sample purity, as the sample-to-noise ratio can be improved by repeating the NMR analysis multiple times and averaging the resulting NMR spectra. As both the signal-to-noise ratio and the presence of impurity peaks are indicators of the experimental conditions and not a feature of the molecule examined, the background noise of NMR spectra were not considered as sound sources in the context of this portfolio.

*As the background noise is random, but the position of NMR peaks are not, averaging multiple spectra taken consecutively will lead to constructive interference for peak signals and (slower) uncorrelated growth for background noise. When averaging \( n \) NMR experiments, the signal-to-noise ratio is improved by a factor of \( n^{1/2} \).

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Chapter 3. Spin Dynamics

*Spin Dynamics* is a multi-channel acousmatic piece based exclusively on the sonification of hydrogen-1 and carbon-13 nuclear magnetic resonance data (abbr. NMR data). *Spin Dynamics* was created to explore the use of spectroscopic data in electroacoustic music compositions. A methodology for the sonification of hydrogen-1 and carbon-13 NMR spectra was developed, and the results were published elsewhere.\(^4\)\(^5\).*

3.1 Data sources and sonification methodology

3.1.1 An introduction to nuclear magnetic resonance spectroscopy

A full explanation of the principles of NMR spectroscopy is beyond the scope of this commentary. An introduction to the principles of NMR analysis can be found in Appendix F. In short, the chemical shift measured in NMR spectroscopy is an indicator of the chemical environment surrounding an NMR-active atomic nucleus.\(^x\) If the nucleus is surrounded by a high electron density it will have a low resonance shift. Nuclei in environments of low electron density have higher resonance shifts. The magnitude of these resonance shifts can often be predicted beforehand and can be compared with the results of the NMR measurement. NMR spectroscopy is such a powerful tool that commonly the different features of an NMR spectrum will give a chemist enough information to determine the structure of even unknown compounds beyond doubt.\(^+\)


\(^5\) Please see Appendix B for a copy of the published paper.

\(^x\) For a nucleus to be detectable by NMR spectroscopy it must have an uneven proton and/or neutron count.

\(^+\) When registering new compounds, submitting the respective NMR spectrum and a high precision mass analysis is often enough to prove that the proposed compound has been made, a testament to the illuminating powers of both techniques.
Hydrogen-1 and carbon-13 NMR spectroscopy are the most commonly used types of NMR measurements with hundreds of thousands of spectra of molecules already analysed and available online. As a very basic analogy of an NMR measurement, we can think of molecules as loose guitar strings which, by themselves, make no sound. Only when those molecules are put into a magnetic field and hit by a radio-pulse (analogous to fixing a guitar string to a guitar and plucking it), will they emit a signal. For 1H-NMR and 13C-NMR spectroscopy, the difference between these signals and a reference signal is recorded. The recorded signal, also known as Free Induction Decay (FID), typically lies in a range of 0 – 20000 kHz and can be audified directly. It is also possibly to analyse the FID signal and sonify the peak data via additive synthesis as seen in figure 3.* Unless stated otherwise, NMR data was sonified using additive synthesis, removing the background noise induced by the NMR measurement, as discussed in chapter 2.4.2.

![Sonification scheme for the transformation of NMR data to sound, as described by Morawitz.](Image)

* A summary of the code written for spectroscopic data sonification can be found in Appendix F.

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3.1.3 Characterisation of obtained sound morphologies

As described elsewhere, audified 1H-NMR spectra and spectra sonified via additive synthesis resemble most closely the sound of bells, due to their non-harmonic arrangement of sine waves and their exponential attenuation times of one to five seconds. Depending on the complexity and symmetry of a molecule, 1H-NMR spectra can contain just a few or up to many hundreds of sine waves in the range of 0 – 4000 Hz.

Due to their short attenuation times of less than a second, additively synthesized and audified 13C-NMR spectra are more reminiscent of percussive sounds. 13C-NMR spectra of simple molecules quite often only contain 1 - 10 signals, sounding like short sine-wave pulses.

3.2 Structure

For Spin Dynamics, 100 small molecules were selected and their hydrogen-1 and carbon-13 NMR data were sonified. Molecules with interesting structural features were searched for in the human metabolome database. The NMR data was sonified using additive synthesis and FID audification.

As described elsewhere, most of the sounds heard in the composition were transformed using a set methodology: keeping one aspect of the raw molecular sound unchanged, but freely altering every other aspect. The sound material obtained was then arranged, with each section of the music composition highlighting different aspects of the spectroscopic sound material.

0:00 – 2:14 minutes

The composition starts with a direct audification of an ethanol 1H-NMR spectrum, adding overtones over time. The strong pulsing character of the sound material was retained but the timbre was altered by sequentially adding more overtones.

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Towards the end of the section, the pulsing is altered in its frequency for each of the eight speakers individually, adding spatial fluctuations to the texture.

2:14 – 3:30 minutes

The water-like sounds prominent in this section were created by sequentially sonifying random frequency peaks of a highly complex 1H-NMR spectrum: a small selection of the roughly 100 frequency peaks of that spectrum were sustained for a few hundred milliseconds before being followed by a new, random selection of frequency peaks of the same spectrum. At 2:30 minutes, the audification of ethanol is reintroduced but with a changed timbre, leaving only its tremolo-type features intact. Towards 2:53 minutes a new, abrasive sound is introduced, an assortment of high-frequency 13C-NMR sounds that were rhythmically altered via AM-synthesis.

3:30 – 5:15 minutes

The main feature of this section is based on the data of another highly complex 1H-NMR spectrum. Instead of presenting the timbre of the whole spectrum at once, a narrow band-pass filter sweeps through the spectrum's frequencies, exposing a few frequency peaks at a time. From four minutes on, the same NMR spectrum is again swept through using a band-pass filter, additionally transformed using a resonator, giving the resulting sound more bell-like properties.

5:15 – 7:05 minutes

This segment presents short percussive sounds, continuously repeating over an organ-like counterpoint drone. The short percussive sounds are unaltered 13C-NMR sounds with the organ-like drone being created through multiple parallel pitch shifting transformations of the 13C-NMR data.

7:05 – 10:00 minutes

The final section reintroduces previously heard sound material but combines and rearranges them in new patterns. Instead of highlighting a singular feature of an NMR sound, this section explores the interplay of NMR-derived sound material with one another.
4. Inner Resonance

Inner Resonance is a music composition for bass clarinet and electronics. It was created to explore the similarities, the contrast and the interplay between sounds created by solid-state nuclear magnetic resonance sonification, and the sound of the bass clarinet.

4.1 Data sources and sonification methodology

Inner Resonance is an investigation into the interplay of two different sound domains: the sounds obtainable via sonification of solid-state NMR data and the sounds obtainable by playing the bass clarinet. For the creation of Inner Resonance, a library of sounds from both domains was created first. The emphasis during the creation of this sound library was to explore sound creation methodologies for both sound domains that reference features of the other sound domain, respectively. This meant to employ sonification methodologies that have a reference to instrumental performance, using NMR peak data for the tuning of sine wave oscillators triggered by a MIDI keyboard to play short musical phrases in that tuning, as further explained in section 4.1.2. It also meant to record bass clarinet sounds that mirror or allude to spectral features of solid-state NMR, by asking the clarinettist to faithfully reproduce NMR-based sonification sounds using the bass clarinet and by using tunings based on overtone series as basis for the instrumental composition, see sections 4.2 and 4.3.

4.1.1 Solid-state nuclear magnetic resonance spectroscopy

Solid-state nuclear magnetic resonance is a type of NMR spectroscopy in which a chemical sample is investigated in a medium of little mobility, such as crystals or powders. Because the molecules in such a sample are not free to move, detecting directionally dependent interactions between nuclei is a characteristic feature of solid-state NMR. It is possible to minimise the effect of directionally dependent interactions in the sample by spinning the crystal at a certain angle during the NMR measurement. If this spinning is relatively slow, so-called spinning sidebands will occur, as seen in figure 4. These sidebands are equally spaced from one another with the spacing frequency being equal to the spinning frequency of the sample.
Figure 4: A solid-state 1H-NMR signal depicting one signal and its corresponding sidebands.

4.1.2 Sonification of hydrogen-1 solid-state NMR data

Peaks in a solid-state 1H-NMR spectrogram can shift by up to 300 ppm corresponding to ringing frequencies of up to 150 kHz on standard 500 MHz spectrometers. To sonify these spectra, peak frequencies were transposed into the audible range before sonification. The NMR frequency data were divided by factors of 10, 50 and 500* and the resulting sets of frequencies were used as a basis for subsequent sonification procedures (Figure 5).

* Division factors of 10, 50, and 500 were chosen to confine the data to different frequency ranges. A division by 10 spreads the NMR spectrum over the whole audible range. A division by 50 spreads the NMR data over low and mid-frequencies only. A division of 500 transposes the NMR data to bass frequencies only.
Identically to liquid-phase NMR spectra sonification, the noise patterns of solid-state NMR spectra were omitted from sonification, as rationalized in chapter 2.4.2. The frequency sets obtained by transposing solid-state NMR data were subjected to three sonification approaches herein referred to as static, variable, and performative. For a static sonification, the data was sonified with constant and uniform attributes, assigning all sine waves of the additive synthesis the same initial phase and amplitude envelope. In the variable sonification, attributes such as phase, attack, decay, sustain, release, and onset delay of each sine wave was controlled in real-time during the additive synthesis procedure. The performative approach mapped every frequency peak of an NMR spectrum to ascending keys on a MIDI-keyboard and small phrases with the tuning the spectroscopic data were played and recorded. The sound results of all three types of additive synthesis sonification were collected and used for subsequent sound transformations.

4.2 The bass clarinet and sonification

The sound creation stage was heavily guided by Spaarnay’s book ‘The bass clarinet – a personal history’. The bass clarinettist was asked to reproduce selected techniques featured in the book, focusing on multiphonic tremolos, air sounds, harmonic overtone series and short sequences of transitions between them. Particularly harmonic overtone series show similarities with solid-state NMR spectra, as both prominently feature equal frequency spacing (Figure 6).

![Figure 6: Overtone series on A2. In this series, adjacent notes are 110 Hz apart.](image)

Besides the sound creation methods outline above, short arrangements of NMR-based sound were played to the bass clarinettist for her to reproduce them as truthfully as possible using the bass clarinet only. These short NMR-inspired bass clarinet phrases, as well as the sound mentioned above were then used as basic building blocks for the bass clarinet composition.

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4.3 Structure

The score can be found in appendix D. Please note that the score includes an optional part (1:00 – 1:20 minutes). The recording submitted is the premiere of *Inner Resonance* and omitted this optional section. As such, timings in the score and timings in the recording will differ by at least 20 seconds. Additionally, the timings indicated in the score are only guidelines and can vary substantially for each performance. The timings below refer to the music piece submitted in the portfolio, and in brackets the timing as stated in the score.

**0:00 – 1:10 minutes (0:00 – 1:30 minutes in score)**

The piece starts with various transitions of held notes into glissandi and flutter tongues. The amplitude of the accompanying NMR sounds* is tied to the bass clarinet amplitude via an envelope follower. NMR sounds are only heard while bass clarinet is playing. The influence of the envelope follower is lessened over time and towards the end of the first minute sounds of both sound domains coexist independently from one another.

**1:10 – 1:30 minutes (1:30 – 2:05 minutes in score)**

This section explores the interplay of the instrumental and NMR sonification spectromorphologies in the temporal domain featuring a series of onset-termination gestures. Over a series of consecutive gestures, the onsets are created from either bass clarinet or NMR sound material and then combined with a termination from either the opposing or same sound domain.

**1:30 – 2:30 minutes (2:05 – 3:10 minutes in score)**

This section uses counterpoint of gestural material from both sound domains to explore the interplay of instrumental and NMR sound material. Shifting timings between the start of instrumental and NMR sounds are implemented to create a variety of textures.

**2:30 – 4:00 minutes (3:10 – 4:35 minutes in score)**

This segment is built around tonal scales based on harmonic overtone series. Sounds of the bass clarinet are artificially prolonged using reverb tails. Different held notes of the bass clarinet merge into one texture that is first contrasted by rhythmic NMR sounds and later complemented by a continuous NMR sound texture.

* For brevity, the term 'sounds created from sonification of solid state 1H-NMR data' is abbreviated to 'NMR sounds' in this section.
4:00 – 6:00 minutes (4:35 – 6:00 minutes in score)

The last segment features a sequence of NMR crescendos contrasted with rhythmic gestural key clicks and later complemented with textural multiphonic tremolos. After the last crescendo a final texture emerges: a weighted convolution\(^{53}\) (i.e. a spectral merge) combining the timbral qualities of the bass clarinet and the NMR spectra into one new unified sound texture.

5. Quantum

*Quantum* is a virtual reality experience that depicts stylised molecules in a simulated environment. The behaviour of those molecules is determined by chemical data and theoretical models: atoms provide audible feedback according to their nuclear ringing frequencies and molecules arrange in space according to the valence shell electron pair repulsion model. Through hand sensors, participants can reach out into virtual space and interact with and distort the molecules on display monitoring the auditory and visual response of the virtual chemical compounds. The visual design of *Quantum* focuses on minimalistic and abstract visuals and aims to encourage participants to focus their attention on the sonic responses of their actions (Figure 7). These sound responses are at first direct sonifications of nuclear spin data but upon continued activity of the user, more complex sound material and short compositional phrases emerge. *Quantum* explores the use of interactivity, immersion, and visual cues as synergists to spectroscopic sonification.

*Figure 7: Quantum, screenshot.*
Quantum was first shown at Laboratory, Spokane, Washington and was later presented at the Workshop for Sonic Interaction in Virtual Environments and published via IEEE Xplore.\textsuperscript{54} The published paper is included in Appendix B. The paper covers design and implementation of the auditory and visual aspects of the installation whereas this chapter focuses on peripheral aspects of the installation, such as thoughts on the crossover between game audio, electroacoustic composition and composition structure.

5.1 Data sources and sonification methodology
Quantum builds on the sonification procedure previously developed and presented in Chapter 3.1 and elsewhere.\textsuperscript{55} The sonification procedure is expanded by incorporating not only hydrogen-1 and carbon-13 NMR data, but phosphorus-31, nitrogen-15 and oxygen-17 NMR data for sonification (Table 2).

<table>
<thead>
<tr>
<th>Nucleus Type</th>
<th>Typical frequency range in kHz\textsuperscript{*} \textsuperscript{56}</th>
<th>Number of spectra available online\textsuperscript{57,58}</th>
<th>Typical signal attenuation time in s\textsuperscript{59}</th>
</tr>
</thead>
<tbody>
<tr>
<td>1H</td>
<td>0 - 5</td>
<td>&gt; 100 000</td>
<td>2 - 6</td>
</tr>
<tr>
<td>13C</td>
<td>0 - 15</td>
<td>&gt; 50000</td>
<td>0.1 - 6</td>
</tr>
<tr>
<td>15N</td>
<td>0 - 15</td>
<td>&gt; 8000</td>
<td>0.1 - 3</td>
</tr>
<tr>
<td>17O</td>
<td>0 - 20</td>
<td>&gt; 100</td>
<td>0.02</td>
</tr>
<tr>
<td>31P</td>
<td>0 - 2</td>
<td>&gt; 100</td>
<td>0.1 - 0.25</td>
</tr>
</tbody>
</table>

Table 2: Comparison of NMR spectra of selected nuclei.

\textsuperscript{*} Frequency range of common functional groups measured on a 500 MHz spectrometer.


As described in the corresponding paper, by presenting molecules as 3D entities in virtual reality, frequency data can be assigned to their corresponding nuclei of origin, virtually spatialising the auditory display (Figure 8).

![Figure 8: The ringing frequencies of propanol measured using a 500 MHz spectrometer. Frequency data assigned to their nuclei of origin.](image)

5.2 Sonification and virtual reality

5.2.1 Setup and controls

*Quantum* is a virtual reality environment presented via an Oculus Rift VR headset. Participants interact with the virtual environment using a Leap Motion hand tracker that translates their hand movements into virtual space. Participants can move around in virtual space using hand gestures or by using a wireless controller (Figure 9).

![Figure 9: Setup, including VR headset, a leap motion tracker, a standard Xbox controller and various screens displaying the virtual environment.](image)

5.2.2 Thoughts on interactive sonification in virtual reality

The sonic information encrypted in sonification works is understood and interpreted best if the listener had an introduction and, ideally, training sessions with the auditory display. This procedure helps the listener to understand the link between sound features and corresponding data trends. If the aim of a sonification work is to communicate data

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relations through changes in sound parameters, showcasing sonification works as part of an electroacoustic concert is arguably one of the more challenging modes of presentation. In a concert, a piece is generally only played once, and no time is allotted to explaining the relation between data and sound. This results in the need to provide the missing context either through paramedia, visual iconography or narration. *Quantum* explores an alternative mode of presentation by incorporating the auditory display into an audio-visual, immersive and interactive virtual reality installation. Presenting sonification works as such a closed perception-action loop offers the audience the opportunity to explore the display at their own pace and learn, via interaction, more about the datasets and the underlying rules of molecular behaviour.

5.3 Structure

*Quantum* can repeatedly cycle through the four stages outlined below. Stages to include at any given showing of *Quantum* can be set from its main menu. Stages 1 and 3 are described in more detail elsewhere.\(^{62}\)

**Stage 1**

The aim of Stage 1 is to familiarise the participant with the visual and auditory logic of the work, and to establish a link between the visual and sound aesthetic and the information they represent. This stage establishes that every coloured sphere represents a different type of atom and that their sonic response is specific to their atom type. Small molecule-specific musical themes are played once a participant has interacted with most atoms of a given molecule, encouraging the participant to find as many different molecules as possible. All sounds heard in this section are unaltered sound materials created through sonification of NMR data of the corresponding atoms. The participant is given the task to interact with a set number of molecules. If successful, the next stage of the composition is initiated.

**Stage 2**

The molecules found during stage 1 are spawned in a circle around the participant. Interacting with these molecules now elicits more sophisticated sound patterns: atoms can be switched on or off to play sounds, and the sound response of certain atoms will change

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depending on the participant’s hand velocity and gesture, giving the participant the chance to be the conductor of a small molecular ensemble. Participants can interact with the surrounding molecules as long as desired. Upon leaving the designated interaction area, stage 3 is initiated.

**Stage 3**

This is the main part of the virtual reality experience and described in greater detail elsewhere. This stage is based on the idea of energy states, with every molecule either existing in a low or high energy state. Upon prolonged user interaction, molecules can jump from a low to high energy state and their sound response changes accordingly. If enough molecules are in a high energy state at any given time, more complex sound patterns and material are introduced. After the participant has interacted with 5 – 10 molecules (the exact number depending on the settings made in the main menu), stage 4 is initiated.

**Stage 4**

A short reprise of the sound material heard in section 1 in a visually sparse environment.

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64 Ibid.
6. Darkest Hour

Darkest Hour was commissioned by the Instigate Arts Collective and the People’s History Museum (PHM) as part of Manchester After Hours 2016. Manchester After Hours is an annual city-wide event where museums, galleries and cultural centres stay open for evening movies, music and art performances. The PHM houses a wide variety of material, mostly related to the Labour Party as well as the Communist Party of Britain, in form of correspondence letters, party-affiliated flyers and newspapers. Darkest Hour is a sound-centric multimedia piece based on material stored in the PHM archives, specifically material concerning the response to the refugee crises during the First and Second World War. In the piece, archival materials are contrasted with audio snippets from the current refugee debate, tracing similarities and differences in the refugee debate over the decades. The work is a collaboration between Falk Morawitz (tonal sound transformations, creation of textural music material, and creation of visual material) and Guillaume Dujat (interviews, audio recordings, and vocal sound transformations).

6.1 Data sources and sonification methodology

The library of recordings and tonal sequences were supplemented by sound material created from chemical and spectroscopic sonification. The piece uses sonifications of 1H-NMR data of mustard gas (Figure 10) created via the sonification methodology described in chapter 3 and elsewhere.65

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The piece additionally uses chemical reaction dynamics as data source, specifically computer simulations of the Belousov-Zhabotinsky reaction. The Belousov-Zhabotinsky reaction is a non-linear chemical reaction in which the concentrations of certain chemicals do not decrease or increase steadily, but oscillate. Belousov-Zhabotinsky reactions have been studied for their chaotic behaviour* and different theoretical models for its simulation have been proposed. Figures 11 and 12 plot the ratio of starting material to reaction product over time for different initial conditions calculated using the Györgyi-Field model, resulting in various periodic and non-periodic patterns. The data gained by these simulated reactions were mapped to control a variety of parameters on sound transformation devices such as granular synthesisers, delay lines, and gates.

* Chaos in this case does not mean a random behaviour, but rather that the development of the system is highly sensitive to its initial conditions.

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6.2 Additional sound sources

*Darkest Hour* is predominantly based on material found in the PHM archives, especially material filed under 'Belgian refugees',71 'air raids and children',72 and 'the labour leader newspaper'.73 Selected texts from the archive were read out by a voice actor and recorded. Interviews were recorded with elderly Basque people inviting them to share their memories of the Second World War. Sound snippets of speeches on the refugee situation of contemporary political figures were incorporated as well as recordings of planes, railroads, and marching soldiers. A full list of external sound sources can be found in Appendix I.

6.3 Tonal progressions

Tonal structures in *Darkest Hour* were inspired by the tonal progression in *Hymn*,74 a short song in aid of the Belgian relief, of which the score was found in the archive.

6.4 Sonification and moving images

The visual material consists of pictures taken from the PHM archives, as well as public domain war footage and speeches of political figures. All video sources are credited in appendix I. The visuals were treated with data created from the Belousov-Zhabotinsky reaction. A modified version of Zammataro’s algorithm75 was used to simulate the localisation of starting material (white) and reaction product (black) in a 2D space (Figure 15). The resulting line drawings were then overlaid with the chosen video footage to achieve effects as seen in figure 13, 14 and 16.

![Figure 13](image1.png)  ![Figure 14](image2.png)

**Figure 13:** The Belousov-Zhabotinski line drawings as seen in *Darkest Hour*.  **Figure 14:** Overlay of Belousov-Zhabotinski lines with footage of marching soldiers.

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71 People’s History Museum archive, LP/WNC/3/1.
72 People’s History Museum archive, LP/WNC/2/2.
73 People’s History Museum archive, KV 2/1916 (1913-1915).
74 H. Newbolt and H. Kibart, "Hymn. In The Time Of War And Tumults" (Manchester), People’s History Museum archive, WNC 3/1.
Figure 15: A Max/MSP algorithm analyses 1 pixel-wide cross sections of an idealised Belousov-Zhabotinski reaction and expands them to black and white lines.*

Figure 16: Belousov-Zhabotinski lines as part of the visual transformation. The words seen on screen are derived from material stored in the PHM archives.

* See file *:\2Supplementary\VideosAndPresentations\How_to_turn_chemical_data_into_visuals.mp4 for a video demonstration.
6.5 Structure

0:00 – 3:55 minutes

This section focuses on the display of current dialogue on the refugee crisis, creating a cacophonic choir in which the voices of compassion are periodically drowned out. Tonal textures inspired by *Hymn* accompany this section but are heavily transformed, as if to ask what has happened to the compassion of the past.

3:55 – 7:10 minutes

The second section focuses on the representation of war, including sounds and video material reminiscent of air strikes, marching soldiers and tank fire. This section additionally features sound material created via sonification of 1H-NMR of mustard gas.

7:10 – 11:30 minutes

The third section focuses on refugee stories shifting the dialogue from impersonal casualty numbers back to individual human tragedies. This section includes an almost unchanged quotation of *Hymn* (9:20 – 9:40min) as the climax of the piece.
7. Finland, as experienced by the Sea

*Finland, as experienced by the Sea* utilises sonified infra-red, nuclear magnetic resonance and oceanographic data as sound sources, combined with field recordings taken on Örö Island, a small uninhabited island in the south-west of Finland. The structure of the piece arises by mapping the changes in pollution concentrations in the Baltic sea from 1960 to 2010 to different sound reproduction parameters, resulting in a data-driven eight-minute acousmatic composition.

7.1 Data sources and sonification methodology

7.1.1 Pollution problems in the Baltic sea

Due to its comparatively small connection with the North Sea, the Baltic Sea is an area especially prone to pollution, as its water masses cannot readily mix with the ocean and pollution cannot be diluted easily. In the latest report of the Baltic Marine Environment Protection Commission, out of 104 coastal data collection locations, 98 had chemical pollution levels high enough to have an impact on the local underwater ecosystem. The pollution types threatening the Baltic can broadly be categorised into organic compound waste, nitrates and phosphates, heavy metals, and radioactive pollution.

7.1.2 Data sources

The Baltic is regularly monitored for numerous pollutants and this data is made available by the Baltic Marine Environment Protection Commission. For *Finland as experienced by the Sea*, oceanographic data and datasets for the concentration of the pollutants nitrate and phosphate, as well as caesium-137 were obtained using the web-interface provided.

* A more detailed description of pollution trends in the Baltic from 1940 – 2010 can be found in appendix J.

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77 ”HELCOM, Hazardous Substances In The Baltic Sea”, *Balt Sea Environ. Proc.*, 120B (2010).
78 Ibid.
Data for the organic compounds PCB and DDT were taken from Bredhult et al., while plastic data trends were taken from Rummel et al.  

7.1.3 Structure

*Finland, as experienced by the Sea* consists of five sections: a vocal section followed by four movements based on the sonification of different pollution types. The structure of the piece is fully determined by underlying data trends: a custom-made sequencer (Figure 17) sequences pollution data from 1960 to 2010 and plays sound material relating to each pollution type more frequently or louder if their concentration is high in a given year. It stops the playback of the sound material once the concentration of the corresponding pollutant falls beneath a previously defined threshold. The four pollution types used for *Finland, as experienced by the Sea* peak in different years (Figure 18) and the rise and ebb of pollutant concentrations is reflected in the rise and ebb of four different types of sound materials (Figure 19).

![Figure 17](attachment:image.png)

*Figure 17:* Screenshot of a section of the custom-made sonification sequencer, displaying a data display window in the upper half of the screen and two sound modules in the lower half. A documentation of the sequencer and its modules can be found in Appendix K.

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84 Carolina Bredhult and others, "Study Of The Relation Between The Incidence Of Uterine Leiomyomas And The Concentrations Of PCB And DDT In Baltic Gray Seals", *Reproductive Toxicology*, 25.2 (2008), 247-255.

Figure 18: Normalized concentration changes for DDT/PCB, nitrate and phosphate, caesium-137 and plastic pollutants in the Baltic Sea. Data sources referenced in chapter 7.2.

Figure 19: Translation of pollution trends to a compositional structure. Every year of pollution data is compressed to ten seconds of composition.

To separate the four pollution sections sonically, the sound material for each pollutant was based on a different sonification methodology for its creation and structuring, as described in the following pages.
Section A 0:00 – 0:30 min: overture

The only section of the composition that does not involve any kind of sonification. The composition starts with the first verse of *Maame*, Finland’s informal national anthem. In the first verse of the anthem, the preciousness of the Finnish waters and shores are appraised (translation: "No hidden vale, no wavewashed strand. Is loved, as is our native North. Our own forefathers’ earth."87), providing a semantic link to the rest of the composition. Sections of the chorus re-occur throughout the piece, during times of exceptionally high pollutant concentrations.

Section B 0:30 – 4:20 minutes: oceanographic data sonification

Section B is a granular texture that is controlled by oceanographic data from the Baltic Sea, as outlined in table 3 and serves as an accompaniment to sections C – F. The sonification procedure uses oceanographic data to control the pitch and timbre of a sound texture by driving grain length and position of a granular synthesis process. The sample that is granularised starts at a low pitch and gradually increases in pitch over time. Repeated playback of grains from the start of the sample therefore results in a lower pitched texture than via the playback of grains from the middle or end of the sample. The Baltic Sea’s pH value and salinity are mapped to the grain length and number of grains per second, respectively, resulting in small data-driven timbral differences in the sound texture.

<table>
<thead>
<tr>
<th>Data dimension</th>
<th>Sound synthesis parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>temperature [0, 20 °C]</td>
<td>-&gt; grain start position [0, 100%]</td>
</tr>
<tr>
<td>salinity [0, 20 psu]</td>
<td>-&gt; grain duration [0, 1000 ms]</td>
</tr>
<tr>
<td>pH Level [0, 10]</td>
<td>-&gt; grains per second [0, 100]</td>
</tr>
</tbody>
</table>

*Table 3: Parameter mapping of section B. Notation after Hermann.88,*

* Table 3 lists the mapping of data features to sound synthesis parameters and is read as follows: The data feature *temperature* is linearly mapped in the range of 0 to 20°C to the sound synthesis parameter *grain start position* from 0 to 100%. This means that a temperature value of 0 °C sets the grain start position to 0% (the start of the sample). If the temperature value was 10 or 20 °C the grain start position would move to 50% or 100% of the sample length, respectively.

88 Thomas Hermann, "Sonification For Exploratory Data Analysis" (Ph.D thesis, Bielefeld University, 2002).
Section C 0:30 – 2:00 minutes: organic pollution and infra-red spectroscopy data sonification

The sound material used in section C is obtained via sonification of infra-red spectra of polychlorinated biphenyl (short: PCB, figure 20) and dichlorodiphenyltrichloroethane (short: DTT, figure 21) using the sonification methodology developed by Delatour.\(^8^9\) The sonification methodology involves the analysis of relevant infra-red absorption spectra (Figure 22) and subsequent sonification via additive synthesis. The resulting sound files were stored in the probability-based sample trigger of the data-driven sequencer and their trigger probability was linked to the DDT and PCB concentrations in the Baltic (Table 4).

![General structure of PCB.](image)

**Figure 20:** General structure of PCB.

![Structure of DDT.](image)

**Figure 21:** Structure of DDT.

![Infra-red spectrum of DDT.](image)

**Figure 22:** Infra-red spectrum of DDT.

<table>
<thead>
<tr>
<th>Data dimension</th>
<th>Sound synthesis parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCB concentration [μg/g lipid weight]*</td>
<td>sample trigger probability [0, 100%, every 0.1 seconds]</td>
</tr>
<tr>
<td>DDT concentration [μg/g lipid weight]*</td>
<td>sample pitch [-2oct, +2oct]</td>
</tr>
</tbody>
</table>

**Table 4:** Parameter mapping for section C.

* The concentration of organic pollutants is commonly determined by measuring its accumulation in the fatty tissues in fish and sea mammals, hence the units.

---

Section D 2:00 – 3:45 minutes: eutrophication and NMR sonification

The sound material in section D is created via 15N and 31P-NMR data sonification of the ions \( \text{NO}_3^- \) and \( \text{PO}_4^{3-} \), respectively. Both spectra contain only one signal each, resulting in a total of just two sine waves. Instead of outputting both sine waves directly, they are routed to amplitude-modulate each other. The sine wave based on 15N-NMR data plays constantly while the 31P-NMR sonification sounds are triggered depending on their concentration (Table 5). To increase the difference in morphologies between section C and D, the sonic output was further transformed using sound distortion and wave-shaping.

<table>
<thead>
<tr>
<th>Data dimension</th>
<th>Sound synthesis parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>nitrate concentration [0, 40 ( \mu \text{mol/L} )] -&gt;</td>
<td>15N-NMR frequency alteration [0%, 10%]</td>
</tr>
<tr>
<td>nitrate concentration [0, 40 ( \mu \text{mol/L} )] -&gt;</td>
<td>AM modulation depth [0.1, 1]</td>
</tr>
<tr>
<td>phosphate concentration [0.18,1.00 ( \mu \text{mol/L} )] -&gt;</td>
<td>31P sample trigger probability [0,100%]</td>
</tr>
<tr>
<td>phosphate concentration [0,1.00 ( \mu \text{mol/L} )] -&gt;</td>
<td>31P sample pitch change [-3 oct, +3 oct]</td>
</tr>
<tr>
<td>phosphate concentration [0,1.00 ( \mu \text{mol/L} )] -&gt;</td>
<td>31P sample pitch change occurrence [0, 80% for each sample trigger]</td>
</tr>
<tr>
<td>nitrate concentration [0, 40 ( \mu \text{mol/L} )] -&gt;</td>
<td>31P sample trigger frequency [5 s(^{-1}), 10 s(^{-1})]</td>
</tr>
</tbody>
</table>

Table 5: Parameter mapping for section D.

Section E 3:45 – 4:20 minutes: radioactive material

Section E uses the clicking of a Geiger counter as a representation of the influx of caesium-137 into the Baltic. The sound of the Geiger counter is one of the few auditory icons that is, through exposure in popular media, widely understood in Western culture without the need for training or explanation.* For section E, the concentration of caesium-137 is mapped to the sample trigger probability, resulting in more frequent clicks at higher concentrations (Table 6).

<table>
<thead>
<tr>
<th>Data dimension</th>
<th>Sound synthesis parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>caesium-137 concentration [0, 500 mBq/L] -&gt;</td>
<td>sample trigger probability [0,100% -every 0.05 - 0.1 seconds-]</td>
</tr>
</tbody>
</table>

Table 6: Parameter mapping for section E.

* One of the next big hurdles for sonification might be to develop a common semantic so that sonifications can be 'intuitively' understood, similar to how visual graphs have a common structure that we have come to understand through years of school training.
Section F 4:20 – 8:00 minutes: plastic

The last section of this piece is based on the recordings of folding and crushing plastic bags and plastic wrappings. The obtained sound material was triggered using the data sequencer with the mapping outline in table 7.

<table>
<thead>
<tr>
<th>Data dimension</th>
<th>Sound synthesis parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>plastic concentration [0, 50%]</td>
<td>sample trigger probability [0, 100%, triggered every 0.05 - 0.1 seconds]</td>
</tr>
<tr>
<td>plastic concentration [0, 50%]</td>
<td>amplitude (0, 100%)</td>
</tr>
</tbody>
</table>

Table 7: Parameter mapping for section F. Plastic concentration measured in percent of fish found with quantifiable ingested plastic residues. Data by Rummel et al.90

7.2 Presentation

Finland, as experienced by the Sea was one of the first pieces in the portfolio to reference extra-musical ideas. Presenting the piece in acousmatic concerts was not satisfying as program notes could only give a hint of the underlying sonification procedures, leaving much of the extra-musical content undelivered. The piece was later presented as part of sonification talks and workshops. The benefit of presenting the piece this way was that data sources and the sonification sections B to F can be discussed in detail and presented individually, before showing the finished piece, making this the preferred mode of presentation (see Appendix L for a selection of slides delivered during these workshops).

90 Christoph D. Rummel and others, “Plastic Ingestion By Pelagic And Demersal Fish From The North Sea And Baltic Sea”, Marine Pollution Bulletin, 102.1 (2016), 134-141.
8. On the Extinction of a Species

“The people of each generation perceive the state of the ecosystems they encountered in their childhood as normal and natural. When wildlife is depleted, we might notice the loss, but we are unaware that the baseline by which we judge the decline is in fact a state of extreme depletion. […] Few people younger than me know that it was once normal to see fields white with mushrooms, or rivers black with eels at the autumn equinox, or that every patch of nettles was once reamed by caterpillars. I can picture a moment at which the birds stop singing, and people wake up and make breakfast and go to work without noticing that anything has changed.” – George Monbiot

On the Extinction of a Species is a 21-minute multi-channel music composition. The piece combines an acousmatic sound world with voice narration to tell the story of the extinction of the passenger pigeon.

The topic of the composition, the eradication of four billion pigeons in the late 19th century, is a cautionary tale: even if the actions of an individual person seem negligible, the collective impact of these actions are enormous. Examining the public mindset surrounding the extinction of the passenger pigeon show striking similarities with the treatment of current and pressing global environmental issues such as global warming, the plastic pollution epidemic and the ongoing mass extinction of species. The unwillingness to acknowledge and act upon the impact of our own actions seems to be just as prevalent now as it was in the 1890s. Presenting a music piece concerned with the mass extinction of the passenger pigeon is therefore not only about a tale of the past, but a reminder of the environmental impact of our own actions.

8.1 Data sources and sonification methodology

*On the Extinction of a Species* uses spectroscopic data of the DNA bases adenine, cytosine, thymine, and guanine as a basis for sonification. The data were sonified using the sonification methodologies previously developed and described elsewhere.\(^\text{92,93}\) The sound material is catalogued in the following chapters using the letter S.

8.2 Additional sound sources

The composition is based on four different sources of sound and their transformations.\(^*\) The four sound types are voice recordings, field recordings, spectroscopic data sonification, and oscillator-based analogue synthesis, further detailed below.

Symbol nomenclature:

- **X** – a capital letter denotes a main sound type, if there is more than one sub-type for a given main type X they will have subscript indices, e.g. \(X_M, X_N\)

- **\(X^T\)** – sounds denoted with a superscript ‘T’ created via transformation of sound X. Transformed sounds based on a sound sub-type keep their subscript, e.g. \(X^T_M\) is based on \(X_M\)

*Voice (index: V)*

- **V** – text-to-speech narration and vocoder transformation

- **\(V^T\)** – Voice transformation inspired by speech created by neural networks,\(^\text{94}\) with focus on syllable re-arrangement

*Field and nature recordings (index: FR, B)*

- **FR** – field recordings (ambience, containing no bird calls)

- **BC** – bird calls (band-tailed pigeons\(^*\) and song-birds)

\(^*\) For reference, an example of each sound type can be found on the USB drive under *:\Supplementary\SoundExamples_SoundReferences\ExtinctionSoundReferences.

\(^*\) The band-tailed pigeon is the passenger pigeon’s most closely related living species.


$B_F$ – a pigeon swarm taking flight

$B_C^T$ – bird call transformed via granular synthesis techniques

$B_F^T$ – a transformation that keeps the loudness-contour of $B_F$, but replaced its timbre

**Molecular sonification (index: S)**

$S$ – sonification of $1H$, $13C$, $15N$ and $31P$-NMR data of the DNA bases guanine, cytosine, adenine, thymine, and the phosphate-deoxyribose DNA backbone using the sonification and transformation methodology described in chapter 3: *Spin Dynamics*

$S^T$ – frequency-shifted version of $S$

**Analogue, oscillator-based synthesis (index: A)**

$A_b$ – Analogue synthesis sounds mimicking bird calls based on the synthesis methodology described by Climent$^{95}$

$A_1$ – Noise-based texture 1

$A_2$ – Noise-based texture 2

**Hybrid sounds**

Hybrid sounds were created by combining two or more of the sound types described on the previous page using the outlined synthesis methodologies.

$(V-B)^T$ - continuous analysis of the 10 main frequency peaks of $V$ and $B$ with the subsequent additive synthesis of sine waves at frequencies based on peak data of $V$, $B$ or an interpolation of both

$(S-B_C)^T$ - weighted convolution$^{96}$ of $S$ and $B_C$ to form a hybrid texture

$(S-A)^T$ - gradual changes to $S$ via delay and pitch-shift feedback loops using $A_b$ as voltage control for delay time and pitch shift parameter intensities

$^{95}$ Ricardo Climent, "B is for Bird: A game-audio musical work for resynthesed syrinx", Composition, *Universidade Federal de Uberlandia* *Editora*, 2016.

8.3 Structure

*On the Extinction of a Species* tells the story of life, death, and resurrection of the passenger pigeon. The sound material and its arrangement were chosen to illustrate the chronology of the species’ demise as detailed below and in figure 23.

**Figure 23:** General overview of sound type distribution (see Appendix L for a high-resolution version).

0:00 – 1:20 minutes (corresponding to past times leading up to the 15th century)

The composition starts with unprocessed bird recordings \( B_r \) enveloped by the texture \((S-B_c)\), symbolising a time before the industrial revolution with nature less strongly impacted by human activity.

1:20 – 4:45 minutes (15th century – 1750)

The unprocessed bird sounds are gradually fading away and are replaced with processed bird calls \( B_cT \) symbolising how birds are adapting to the ever-expanding human presence.

4:45 – 6:50 minutes (1750 – 1900)

Starting with sparse spectral content, but eventually building up towards a spectrally rich sound, the texture \( A_2 \) symbolises ongoing industrialisation. The short gap in the texture at 6.45 minutes links to the end of the 19th century, when the last passenger pigeons were killed. After 6.45 minutes, almost no bird recordings are heard in the composition.
6:50 – 10:00 minutes (1900 – now)

The noisy textures $A_1$ and $A_2$ grind along as a symbol of the ongoing industrialisation. Around 9.30 minutes the textures transition into the only field recording of the piece (FR) symbolising the arrival in the present time. The field recording contains almost no bird sounds, symbolic of the deprived state of our ecosphere.

10:00 – 14:40 minutes (now – near future)

This section of the piece is based on the project 'Revive and Restore': a venture led by conservationists and scientists to revive (or more correctly: de-extinct) and re-introduce passenger pigeon-type birds back into the wild. The idea behind 'Revive and Restore' is to fully determine the passenger pigeon's DNA and use that information to selectively change DNA of germ-lines in band-tailed pigeon so the birds developed from those germ lines becomes more and more like the passenger pigeon, mimicking a human-guided, accelerated evolution process.

The sounds heard in this section are transformations of sounds made via NMR data sonification of DNA strands (sound S), alluding to the first step of 'Revive and Restore': the comparative analysis of band-tailed pigeon DNA with passenger pigeon DNA to find the most promising DNA sequences for subsequent alteration.

14:40 – 17 minutes (intermittent future)

The 'resurrection process' of the passenger pigeon.

When thinking about the possibility of resurrecting long lost species, we must ask ourselves how the environment will react to the re-introduction of such animals. Will the ecological niche they once inhabited still be reserved for them or will a re-introduction of a long-lost species be no different to the introduction of an invasive species? Will the resurrection be a triumph or a disaster?

The composition aims to follow the suspense of that moment introducing an imposing and triumphant sound texture. However, in the story the resurrection process fails, and the sound texture disintegrates. Sounds heard in this section are mostly created via running

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DNA data sonification sounds $S$ through an effect-and-feedback loop over many iterations until most of their original sound characteristics are transformed and unrecognisable (sound $(S-A)^T$).

17 – 21 min (far future)

What will be left if we cannot introduce extinct species back into the wild? The composition ends with a notion that the future of conservation and remembrance might lie in the creation of virtual realities in which interactive memorials of ecosystems of old might be preserved. This section introduces the sound family $V^T$ a broken up and 'glitched' version of the original narration $V$. Unlike $V$, $V^T$ is not confined to the centre speaker but spreads over all seven loudspeakers, breaking the barrier between narrator and its environment.

8.4 Acousmatic storytelling and sonification

The piece is situated within the realm of acousmatic storytelling. According to Amelides, the prime focus of this subgenre of acousmatic composition is not the exploration of the timbral and gestural quality of sound objects and their transformation in time, but the creation of a hybrid drama.98 For Amelides, this hybrid drama is created through the interplay of a voice narration and a composed sound world. Many pieces belong or can retroactively be assigned to the realm of acousmatic storytelling. The combination of acousmatic storytelling and sonification is less common even though the importance and benefits of storytelling for fields such as data communication or data visualisation are well documented.99,100 It stands to reason that the employment of acousmatic storytelling in sonification works can improve the effectiveness of the latter at communicating data. *On the Extinction of a Species* explores nuances of acousmatic storytelling to tell a story, but also to explain sonification procedures as they are heard. A more thorough investigation of the combination of sonification and acousmatic storytelling in *On the Extinction of a Species* has been published elsewhere.101

* Examples include Westerkamp's *Kit's Beach Soundwalk* or Francis Dhomont's *Figures*.

100 Thomas Erickson, "Design As Storytelling", *Interactions*, 3.4 (1996), 30-35.
9. 56Fe

56Fe is a nine-minute acousmatic composition that uses sound recordings of steam vents, struck metal, and working machinery to evoke links to the Industrial Revolution and to invite the listener to ponder their relationship with their industrialised environment. Besides sound recordings, the composition uses sounds created from the sonification of electron orbital energy data for water and iron. 56Fe was first shown as a sound art installation in London in July 2018 (Figure 24) and later adapted for a concert hall setting.*

![Figure 24: Picture of the 56Fe sound installation. Participants were asked to enter a small darkened enclosure. Loudspeakers were hidden within the folds of the textile walls in proximity to the listener, creating a sense of immediacy and intimacy.](image)

9.1 Data sources and sonification methodology

The piece is based on sound material related to iron and water, using recordings of struck metal and steam vents. Complementing this sound library are sonifications of iron and water orbital energy level data.

* A copy of this written chapter is usually supplied to the audience as “extended program notes” where feasible, to supply additional information about the composition.
9.1.1. Water orbital data sonification

Water is a covalently bound molecule and the orbitals of oxygen and the two hydrogen atoms merge to create an array of new orbitals at discrete energy levels (Figure 25, 26). These binding energies were translated to frequencies* and scaled. The scaled frequency values and their relative intensities were set to control a series of bandpass filter frequencies and their relative gains, respectively. Each filter was fed with white noise and the outputs of all filters were summed to form the sonification result.

* Energy values in electron volts (eV) and can be converted to frequencies using Planck’s equation:

\[ E = \frac{h \nu}{e} \]

With \( E \) being the energy level of the electron orbital, \( h \) being the Planck constant, \( \nu \) the corresponding frequency and \( e \) the electron charge. For example, the binding energy of orbital 1b₂ is 12.6 eV, which interacts with light at a frequency of \( \frac{E}{h} = 3050 \text{ THz} \).

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Figure 25: Orbitals of oxygen (red) and hydrogen (blue) re-combine when forming H₂O, leading to new hybrid orbitals (green). Orbital energies in electron volt (eV), computed by Ning et al.¹⁰³

Figure 26: Ionisation spectrum of water measured at an impact energy level of 1200 eV, computed by Ning et al.¹⁰²

¹⁰³ Ibid.
9.1.2. Iron orbital data sonification

In metallic iron, orbitals mix just as in water molecules, but because iron metal consists of a high number of atoms, the energy gaps between individual orbitals of the same type become negligible and continuous energy bands are formed (Figure 27), resulting in a broad set of electron energy distribution (Figure 28).

Figure 27: When two or more atoms interact, their orbitals will form new, mixed orbitals above and below the energy levels of the original orbitals. If enough atoms interact, the gaps in energy between these orbitals become negligible and energy bands are formed.

The energy distribution data of electrons in metallic iron (figure 9.5) were sonified exactly like the orbital energy data of water, by scaling and assigning each energy peak to control the frequency of a series of bandpass filters. White noise was run through each filter separately and their outputs were summed according to their relative energy peak amplitudes.

Figure 28: Energy distribution of electrons in metallic iron, data from Dronskowski\textsuperscript{104,105}


9.1.3 Sound characteristics and sonification procedure

56Fe revisits the idea of using reference sounds to help contextualise the sonification sounds. In addition to using real-world reference sound material (e.g. the sound of a passing train), 56Fe employs auditory icons. Auditory icons mimic real-world sounds to encode data or represent processes, e.g. the sound of water filling a glass representing a copying process on a computer, or the sound of crumpling paper when moving computer files into an operating system’s trash bin.¹⁰⁶

In the sonification of water’s and iron’s electron energy distributions (Figure 26 and 28) the bandwidth (Q) of each bandpass filter can be adjusted, as well as its amplitude envelope. Narrow bandwidths and exponential attenuation envelopes result in bell-type sounds, whereas large bandwidths and linear attenuation will result in sounds similar to steam released from steam vents (Figure 29).

![Figure 29: Spectrograms of sonifications of iron electron energy level data for various bandpass filter widths.](image)

9.2 Structure

Like other acousmatic pieces in the portfolio, 56Fe explores the combination of different sets of sound material in each of its sections. The sound arrangement within a section and the arrangement of the music structure follow aesthetic and compositional concerns. No data-driven structure was imposed. Two main aspects that were explored in this piece are the placement of sonification sounds in space and in time, with sound material being crafted to sound far away or very close, and sections that either have highly dense sound material or contain almost no sounds at all.

0:00 – 1:50 minutes

The section starts with the introduction of sound motifs that will recur throughout the piece: a metallic bell made via sonification of water binding energy data, a drone based on the sonification of iron binding energy data (Figure 29), and the sound of passing trains. This section features iterations of mixed gestures in which the arrival and departure parts of the gestures are each based on one of the three sound motifs, but not necessarily the same one.

1:50 – 3:10 minutes

This part of the composition is an exploration of the positions of sounds in space, with the bell-type sound moving in and between panoramic, proximate, and distal composition space.

3:10 – 4:10 minutes

The gesture of the passing train is re-introduced again as departure or arrival halves of multiple mixed gestures. The gestural material in the first half of this section is combined with a low-frequency drone. The second half features contact microphone recordings of vibrating train tracks.

4:10 – 6:15 minutes

This section explores the fluidity between gestural and textural features of orbital energy level data of iron that is sonified and sculpted to resemble steam escaping from steam vents.

6:15 – 9:00 minutes

The last section of the piece reiterates and elaborates on previously introduced sound material. Sounds from the composition, such as the bell-type sound, steam vents, passing trains, and the sonification drone are explored via a variety of sound transformations including recursive effect loops.
10. Conclusions

In seven electroacoustic compositions, this portfolio investigated the sonification of spectroscopic data and the use of spectroscopic sound in electroacoustic music composition. The investigation followed three lines of inquiry in parallel, as detailed in the sub-chapters below.

10.1 Aesthetic implications and sound affordances

The portfolio examined the inherent features of the sounds obtained via audification and sonification of spectroscopic data, and how these sound features influence or mandate subsequent sound transformation and arrangement decisions. *Spin Dynamics* and *Quantum* examined the morphology of spectroscopic sound and its impact on sound transformation and arrangement in compositions. The interactions of spectroscopic sound with instrumental (*Inner Resonance*), environmental (*Finland, as experienced by the Sea*, and *On the Extinction of a Species*) and industrial soundscapes (*56Fe*) were examined as well.

10.2 Paramedia and modes of information communication

The portfolio explored how different types of paramedia and modes of presentation can be utilised to supply the audience with necessary context for the interpretation of the sonification works. Different types of paramedia were employed for different pieces. If a compositional work was presented multiple times, it was presented with different paramedia each time, if possible. Types of paramedia that were explored are concert program notes (*Spin Dynamics, Finland as experienced by the Sea, On the Extinction of a Species*, and *56Fe*), spoken introductions (*Spin Dynamics, Inner Resonance*), explanatory videos (*Quantum*), presentations as part of artist talks (all, but especially *Finland, as experienced by the Sea*), and presentations in thematic art exhibitions (*56Fe*).

The portfolio also explored the incorporation of visuals (*Quantum*), reference sounds and auditory icons (*Finland as experienced by the Sea, On the Extinction of a Species, and 56Fe*) as well as voice narration (*On the Extinction of a Species*) for the communication of context.
10.3. The incorporation of extra-musical ideas via data sonification

Through different combinations of data sources and forms of presentation, paramedia, multi-media, and sound selection described above, the portfolio also explored the incorporation of extra-musical ideas, including the pollution of the Baltic Sea (*Finland as experienced by the Sea*), the extinction of the passenger pigeon (*On the Extinction of a Species*), as well as noise pollution levels of the contemporary city soundscape (*56Fe*).

10.4. Addressing research questions

The portfolio addressed the research questions as follows.

1. How can the sonification of spectroscopic data act as a creative vehicle and innovator for contemporary electroacoustic compositional practices?

Spectroscopic data have been used successfully to create new sounds. Methodologies for the sonification of a variety of spectroscopic data, including nuclear magnetic resonance, infra-red, light absorption, and core excitation spectroscopy data, have been developed and are described in their respective chapters, including direct audification (*Spin Dynamics*), auditory icons and additive synthesis sonification (*56Fe*), as well as parameter mapping sonification (*Finland, as experienced by the Sea*). The morphologies of the resulting sounds were explored in isolation and in combination with instrumental sounds and field recordings, demonstrating the potential of spectroscopic data sonification in electroacoustic music composition.

Even though audification, as a direct translation of experimental data into sound, is the most ‘direct’ type of sonification for NMR data, additive synthesis was chosen as the main sonification technique, as it offered more control over the attenuation envelope, background noise, and phase information. Additive synthesis kept the NMR data’s most important feature, its timbre, unaltered, making it the ideal sonification technique to balance auditory information display and artistic freedom.

For music compositions exploring the aesthetics of NMR-based sounds, such as *Spin Dynamics or Inner Resonance*, a high number of NMR spectra were sonified and only sounds with subjectively interesting sonic properties, such as tremolo rhythms and timbre patterns, were selected for further processing. Additionally, NMR-based sounds were selected aiming to present a broad range of sound morphologies, analogous to selecting the most
interesting and diverse sound material of studio or field recordings. This combination of strict sonification methodology and artistic sound selection allowed for aesthetically interesting sounds to be presented to the public while keeping the artistic intervention on the sonification process itself to a minimum. After NMR-based sounds were selected for their varying sonic features, these features were elaborated, emphasized, and explored in subsequent sound transformation. This process bears a strong resemblance to electroacoustic compositional practices of exploring sound features and morphologies through their spectromorphological development in compositional space and time. For example, the opening of Spin Dynamics highlights the tremolo-type feature of an NMR spectrum by first spreading the tremolo sound to all 8 channels before slightly altering the tremolo frequency of each channel, resulting in an 8-channel counterpoint movement.

Using sonification-based sounds did impose limits to the extent of permissible transformations of sound material: sound material could not be transformed in ways that completely masked all relationships between sound and underlying data morphologies. It is within this limitation that new forms of expression arose leading to the pieces shown in the portfolio.

Room for exploration was created by combining sonified material with field and instrumental recordings. NMR sounds are of remote surrogacy, whereas field recordings and instrumental recordings operate via first and second order surrogacy, respectively.¹⁰⁷*

This difference in surrogacy created opportunities for sonic exploration in which sonified sounds and non-sonified sounds could complement, mimic, contrast or ignore one another, as explored in Inner Resonance. As most non-sonified sounds show first or second order surrogacy, they are usually abstracted to third or remote surrogacies as part of their spectromorphological investigation. Using sonified sound material enabled a new approach

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* Surrogacy, as described by Smalley,¹⁰⁷ is a descriptive concept that links sounds to their perceived causes. First-order surrogacy describes sonic activity of an apprehended source not normally intended for musical use (e.g. bird song). Second-order surrogacy is reserved for sounds of musical instruments and sounds that are perceived to be produced using performative skills. Third-order surrogacy is used to described sounds with inferred but unknown cause, whereas remote surrogacy refers to sounds with unknown cause or source agent that cannot be inferred.

in using a reverse process: starting with abstract sounds of remote surrogacy and in turn transforming them to bells and steam vents, as heard in $^{56}\text{Fe}$.

2. How does the format, presentation, and paramedia of a spectroscopic sonification work influence its reception and the listener’s aesthetic experience?

As the portfolio is an initial exploration into the use of spectroscopic sonification in electroacoustic composition, it explored a variety of presentation methods instead of focusing on one. The results found are therefore only a first indication of the effectiveness of spectroscopic sonification and not a conclusive set of recommendations.

Reflecting on the portfolio, the presentation of spectroscopic sonification as part of an interactive audio-visual installation ($\text{Quantum}$) has been shown to influence the reception of spectroscopic sonification. This type of presentation enabled the audience to explore the auditory display at their own pace. It also involved sonic interaction loops (in this case closed perception-action loops), encouraging the audience to modify molecular shapes and listen to the sonic results. These interactions offer the possibility to interact more deeply with the auditory display and gain a deeper appreciation of the underlying physical phenomena. The notion that interaction is an integral and possibly even the most important part of the sonification of molecular properties in virtual space has been proposed in the context of educational chemistry programs before and appears to be equally valid in the context of electroacoustic music composition.*

Another mode of presentation that has been shown to be effective at furthering the understanding of a composition based on spectroscopic sonification is its presentation as part of or after a workshop or a lecture. Portfolio pieces that were presented as

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* One difference between educational programs and sound installations is that the target audience of the latter is likely not knowledgeable about the principles of spectroscopic chemistry. It can be argued that one of the biggest flaws of $\text{Quantum}$ is that it explained the source of sound in a too-specialised language. This lessened the positive impact of the interaction loop, obscuring the link between sounds heard and the information encoded within those sounds.

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lecture/workshop and concert combinations include *Spin Dynamics, Finland, as experienced by the Sea*, and *On the Extinction of a Species*. The combination of research talks and concerts is common in the field of auditory display and has been adopted as a standard by sonification conferences such as the ICAD\textsuperscript{110} or ZKM’s Strömungen.\textsuperscript{111} This widespread addition of workshops and talks is a testament of its potency for the presentation of sonification work, as laying out the fundamental scientific principles involved and the corresponding sonification methodologies enables the audience to unravel the information encoded in the auditory display.

*Program notes* help to set the context of a music composition but can often, in their briefness, only convey an incomplete explanation of the underlying sonification procedures. As the audience members are most likely not familiar with spectroscopic chemistry, the information gained from program notes is limited.

As exemplified in the portfolio, paramedia carries key supplementary functions for a sonification music piece. It is used to display the sonification methodologies employed and to contextualize the source and meaning of the data used. Paramedia can substitute sonification training sessions and focus the audience’s attention to sonification-related sound properties. In the context of this portfolio, paramedia is an integral part of the compositional process: the portfolio compositions and their paramedia should be considered as a Gesamtkunstwerk that deliver meaning holistically via all media channels employed. This importance of paramedia as integral part of a sonification work is a distinct difference from similar concepts such as Andean’s extramusical narrative.\textsuperscript{112} Paramedia should be considered during the inception and creation of sonification-based compositions and should be developed alongside.

\textsuperscript{110} https://icad.org/ accessed 16.12.2018


3. In what way can socio-cultural connotations towards science be used in sonification-based musical compositions and sound art installations to raise awareness of major environmental and socio-political challenges?

If the allusion to science and mathematics in music composition still inspires awe and wonder in the listener, as it is stipulated elsewhere,\textsuperscript{113, 114} or if the current climate of anti-science populism has left its mark on the reception of science-based music is beyond the scope of this enquiry. What can be said is that the portfolio, by using a mixture of *voice narration, storytelling and thematic reference sounds*, includes pieces that thematise current environmental issues. Together with the techniques presented on the previous two pages, including the presentation of pieces in lecture-and-concert combinations, it can be argued that *Finland, as experienced by the Sea, On the Extinction of a Species*, and $^{56}$Fe are successful in urging the listener to ponder these pressing environmental challenges.

While the pieces are successful at raising awareness, they are successful because of the incorporation of the paramedia and presentation techniques outlined above, and not explicitly because of the use of spectroscopic sonification. For example, if we were tasked how to convey the horror of the First World War, it would be easier to justify the use of a recording of a soldier’s recollection of the battlefield, or the sound of machine guns, than a sonification of spectroscopic data of mustard gas. The portfolio shows that it is possible to create pieces that raise awareness of environmental issues using spectroscopic sonification, but that spectroscopic sonification is not necessarily integral to convey the message. This does not mean that spectroscopic sonification is useless to raise awareness of important issues, but rather that it should be used in a context where the information encoded in the sonification (e.g. the electron energy distribution of a specific molecule) adds meaningfully to the topic at hand.*

\* One such example is the interactive sonification of an HIV enzyme binding site in conjunction with several enzyme inhibitors.


10.5 Research contribution
In addressing the research questions above, the portfolio has explored the use of spectroscopic data in electroacoustic music composition. Even though the audification of NMR data has been known to chemists for decades, this portfolio has explored their use in electroacoustic composition systematically - to the best of my knowledge - for the first time. The portfolio and written commentary contribute to electroacoustic research by developing methodologies for the creation, transformation, and structuring of sounds made from spectroscopic data. Guidelines for the use of spectroscopic data in combination with paramedia, other media, forms of presentation, and voice narration were developed and presented.

10.6 Future work
Many aspects of the use of spectroscopic data in acousmatic music composition are still unexplored. The most promising avenues of future work will likely follow one of three lines of inquiry: the sonification of yet unused types of spectroscopic data, a refinement of the use of spectroscopic data in interactive sound installations, and the in-depth exploration of storytelling and voice in combination with spectroscopic sonification, as outlined below.

10.6.1 Unexplored spectroscopic data types
This portfolio focuses on the use nuclear magnetic resonance data of the nuclei hydrogen-1, carbon-13, oxygen-17, nitrogen-15 and phosphorous-31. While these are the most commonly used nuclei, almost any other element in the periodic table has NMR-active nuclei as well (Figure 30).

![Figure 30: Periodic system of the elements displaying all elements with NMR-active nuclei.](image)
Unlike hydrogen-1 or carbon-13, most of these nuclei shown in figure 30 are quadrupolar, meaning a single nucleus resonates at more than one resonance frequency. Thus, a coupling of a series of quadrupolar nuclei may lead to sophisticated patterns in the NMR data. Other datasets worth exploring include multidimensional NMR spectra. Multidimensional NMR spectra measure the nuclear magnetic resonance of one type of nuclei in respect to another, resulting in two-dimensional and even three-dimensional spectra that show the degree of connection and spatial relationships of nuclei within one molecule.

10.6.2 Modes of presentation
Interactive sound installations - such as Quantum - offer a perfect avenue to let audiences explore a sound display of spectroscopic data at their own pace. While Quantum’s major flaw was the poor explanation of its underlying scientific principles in laymen terms, future interactive sound installations can investigate using explanations employing easily understood metaphors and datasets that are easier to understand (e.g. vibrational and rotational datasets).

10.6.3. Voice and storytelling
On the Extinction of a Species explored the incorporation of voice and storytelling for the contextualisation of spectroscopic sonification. This avenue that can be expanded by the creation of radiophonic pieces that combine storytelling and radio broadcasting. As this format lends itself not only to dissemination on the radio, but also the internet, acousmatic storytelling and radiophonic composition have the potential to engage a much larger audience than localised music presentations.
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77
Appendix A - Glossary

$1H$ is the short form of hydrogen-1.

$13C$ is the short form of carbon-13.

$15N$ is the short form of nitrogen-15.

$17O$ is the short form of oxygen-17.

$31P$ is the short form of phosphorus-31.

Audification is the direct conversion of data points to samples in an audio file or the “direct translation of a data waveform into sound”.\(^\text{115}\) For example, it is possible to audify 24000 data points at a sample rate of 12 kHz as a 2 second sound file.

Carbon-13 describes carbon atoms with a mass of 13u. Unlike the more common carbon-12, which consists of 6 protons and 6 neutrons, carbon-13 has 7 neutrons instead, making it NMR-active.

Chemical sonification is the transformation of chemical data into sound, including all kinds of data derived from chemical systems, such as structural, spectroscopic or thermodynamic data. Chemical sonification is a newly proposed term by the author.

Free induction decay (short: FID) is the signal given off by NMR active nuclei in a strong magnetic field after being subjected to a strong radio-frequency electromagnetic pulse.

Hydrogen-1 is an NMR active nucleus consisting of one proton and no neutrons.

Infra-red spectroscopy is a spectroscopic methodology that uses infra-red radiation to interact with the vibrational states of chemical compounds to determine atomic and molecular bond strengths and other structural features.

Nitrogen-15 is an isotope of nitrogen, containing 7 protons and 8 neutrons.

The nucleus is the positively charged core of an atom consisting of neutrons and protons (except for hydrogen-1 containing no neutrons).

\(^{115}\) Gregory Kramer, Auditory Display (Reading, Mass.: Addison-Wesley, 1994).
Nuclear magnetic resonance spectroscopy uses the interaction of radio-frequency pulses and nuclear spin states to determine the chemical environment of NMR-active nuclei. See Appendix E for more details.

Oxygen-17 is an isotope of oxygen containing 8 protons and 9 neutrons.

Paramedia is a newly proposed term that is used to describe all materials surrounding a creative work that are not part of the work itself. For an acousmatic work, program notes or workshops and lectures about the piece are to be considered paramedia. Paramedia, as a conceptual extension of paratext, shares similarities with Andean’s notion of extramusical narrative,\textsuperscript{116} in that both are umbrella terms to include material surrounding a music composition. Paramedia, with its emphasis on the inclusion of other media than written texts, expands the scope of extramusical narrative, emphasizing that music pieces can be supported by a whole range of media beyond program notes, including videos, banners, workshops, lectures, and more.

Phosphorus-31 is an isotope of phosphorus containing 16 protons and 15 neutrons.

Ppm, or parts per million, is a measure of relative deviation. One ppm is equal to 0.0001%.

Sonification describes the conversion of data into sound to explore or communicate information.\textsuperscript{117}

Spectroscopic sonification, a sub-set of chemical sonification, includes all types of sonification based on spectroscopic data. The term is newly proposed by the author.

Spectroscopy is the umbrella term for a set of analytical methods that scrutinize the interaction of physical matter and electromagnetic radiation to gain insight into atomic and molecular properties such as structure, bond strengths or energy level distributions.


Appendix B – Publications

Publication 1

Publication 2
Falk Morawitz, "An Art-Science Case Study On Sonification And Sound Design In Virtual Reality", 2018 IEEE 4th VR Workshop On Sonic Interactions For Virtual Environments (SIVE), 1, 2018
Molecular Sonification of Nuclear Magnetic Resonance Data as a Novel Tool for Sound Creation

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ABSTRACT
The term molecular sonification encompasses all procedures that turn data derived from chemical systems into sound. Nuclear magnetic resonance (NMR) data of the nuclei hydrogen-1 and carbon-13 are particularly well suited data sources for molecular sonification. Even though their resonant frequencies are typically in the MHz region, the range of these resonant frequencies span only a few tens of kHz. During NMR experiments, these signals are routinely mixed down into the audible frequency range, rendering the need for any additional frequency transpositions unnecessary. The structure of the molecule being analysed is directly related to the features present in its NMR spectra. It is therefore possible to select molecules according to their structural features, in order to create sounds in preferred frequency ranges and with desired frequency content and density. Using the sonification methodology presented in this paper, it was possible to create an acausal music composition based exclusively on publicly accessible NMR data. It is argued that NMR sonification, as a sound creation methodology based on scientific data, has the potential to be a potent tool to effectively contextualize extra-musical ideas such as Alzheimer’s disease or global warming in future works of art and music.

1. MOLECULAR SONIFICATION IN ART, SCIENCE AND MUSIC
In its widest sense, the term molecular sonification includes all procedures that turn data derived from chemical systems into sound. These chemical systems may be single atoms, small molecules, or macromolecules such as proteins or DNA. Although it is possible to sonify some atomic properties in real time, most of the sonification methodology involves turning pre-recorded spectra, or spectral information, into sound.

Scientifically, molecular sonification has been used to analyse large DNA datasets [1], or to find visually imperceptible changes in coupled atomic oscillations [2]. Generally, however, its use in a scientific context is extremely sparse. Contrastingly, molecular sonification has been utilized in various multi-media installations as well as in purely instrumental and acousmatic compositions. In many of those works, molecular systems were sonified ‘indirectly’, for example by assigning musical tones and rhythms to DNA sequence combinations [3], or by assigning musical parameters to size, velocity and positions of atomic clusters [4].

However, molecular systems can be sonified ‘directly’, too, by turning atomic resonant processes measured in analytical chemical experiments directly into sound. Despite a plethora of different spectroscopic methods being available, sources used for direct sonification to date have been almost entirely limited to infra-red spectra. Infra-red spectroscopy measures the vibrational behaviour of atoms and molecules and it has been investigated for its use as a sound source for molecular sonification in theoretical and in applied musical contexts. [5, 6, 7].

One common feature of all these sonification procedures is that artistic choices have to be made during the sonification process: notes or pitches have to be assigned to different chemical features, or choices have to be made on how to transpose infra-red frequencies, typically of many trillions of hertz, into the audible spectrum.

In this paper, nuclear magnetic resonance (NMR) spectroscopy, a standard analytical method in organic chemistry, is presented as a novel and unexplored data source for molecular sonification. In contrast to infra-red spectroscopy, in modern NMR experiments the frequencies of the nuclear signals are converted directly into the audible range during the recording process, enabling a direct translation of data into sound, sometimes described as ‘audification’ [8]. Here, the key physical principles of NMR spectroscopy are introduced. The spectral characteristics of hydrogen-1, denoted $^1$H, and carbon-13, $^{13}$C, NMR spectra are described, and different sonification strategies are discussed. The use of sounds made via sonification of NMR data in acousmatic music composition is contextualized.

2. A MUSICIAN’S INTRODUCTION TO NMR SPECTROSCOPY
Nuclear magnetic resonance is mostly utilized in structure elucidation and validation, as NMR measurements are highly sensitive to structural changes in molecules. For example, Figures 1 and 2, on the next page, show the $^1$H NMR spectra of diethyl ether and methyl n-propyl ether, with the structure formulae $\text{CH}_3\text{CH}_2\text{O}\cdot\text{CH}_2\text{CH}_3$ and $\text{CH}_3\text{O}\cdot\text{CH}_2\text{CH}_2\text{CH}_3$, respectively. Even though the two ethers have very similar structures and contain the same numbers and types of atoms, their NMR spectra are very different.
Figure 1. Simulated $^1$H NMR spectrum of diethyl ether, CH$_3$-CH$_2$-O-CH$_2$-CH$_3$. Note: Conventionally, NMR spectra are drawn with increasing frequency from right to left. In this case 1 ppm equals 500 Hz.

Figure 2. Simulated $^1$H NMR spectrum of methyl propyl ether, CH$_3$-O-CH$_2$-CH$_2$-CH$_3$. Note: 1 ppm $=$ 500 Hz.

It is impossible to accurately explain the mechanisms and principles behind NMR analysis without introducing a vast amount of scientific terms and concepts such as ground state nuclear spin, Larmor frequency or transverse magnetisation. A thorough scientific explanation is beyond the scope of this paper and it is recommended for interested readers to consult M. Levitt’s excellent book ‘Spin Dynamics’ [9]. In simple terms, for a given element with a magnetic nucleus, each atom in a molecule has its own resonance, which is split into a set of resonances with slightly different frequencies if there are other magnetic nuclei nearby. The resonances are measured by placing a sample in a strong magnetic field, then applying a short powerful pulse of radiofrequency and recording the “ringing” of the nuclear spins. Essentially, we can compare the molecules in the sample with tiny bells that are made audible by being hit with a radio frequency hammer.

The signal that is measured is known as free induction decay, or FID, which is subsequently Fourier transformed to yield the NMR spectrum of the sample, as seen in Figure 3. It is possible to convert either the FID or the NMR spectrum into sound, as explained in section 4: “sonification methodology”.

Figure 3. The chemical dopamine and its corresponding $^1$H FID and $^1$H NMR spectrum.

While NMR spectroscopy can detect any atom with an odd number of neutrons or protons, two isotopes especially interesting for sonification are $^1$H (the proton) and $^{13}$C. These nuclei are by far the most commonly used in organic chemistry, with many hundred thousands of datasets available online. The Human Metabolome Database alone hosts spectra for more than 40,000 different chemicals found in the human body [10].

3. CHARACTERISTICS OF SONIFIED NUCLEAR MAGNETIC RESONANCE SPECTRA

3.1 $^1$H NMR

Figures 1 and 2 show typical shapes of a $^1$H NMR spectrum. In order to convert the values normally displayed in units of ppm (deviation from a reference in parts per million) to Hertz, we have to know the reference oscillating frequency of a proton, which in turn is dependent on the magnetic field strength of the NMR machine used and the reference frequency chosen. Here we will assume that the reference frequency is set to zero ppm. In modern NMR experiments the magnetic field strength will very likely correspond to an oscillation frequency of either 500 or 600 MHz, which means that a 1 ppm difference in chemical shift will be equal to 500 or 600 Hertz, respectively.

Knowing this conversion, it can be seen that virtually all $^1$H NMR peaks are situated within the range of 0 – 6000 Hz with most peaks typically lying in between 600 and 4000 Hz.

Depending on which atoms and structures are present in a molecule, frequency clusters will occupy distinct frequency ranges. For example, proton signals associated
with carbohydrates will normally exhibit frequencies around 1 – 3 ppm (500 – 1500 Hz) while unsaturated and aromatic hydrogens, or hydrogens connected to very electronegative atoms, are shifted upwards to 5 – 8 ppm (2500 – 4000 Hz). Figure 4 shows the $^1$H NMR spectrum of ethyl benzene, a molecule with both low and high frequency content, and the assignment of its hydrogens to their corresponding frequency clusters.

The number of signals per spectrum will depend on the complexity and structure of the molecule, and can be as few as one signal or 1000 or more peaks for very complex molecules. Frequency peaks can be spread out over a wide frequency area, as in Figure 4, or concentrated in narrow regions as seen in Figure 5.

$^1$H nuclei are coupled to neighbouring $^1$H nuclei, causing peaks to be split into “multiplets” by what is known as J-coupling. A single resonance is split into a set of slightly different frequencies, up to a few tens of hertz across. In the simplest cases, resonances are split into $N + 1$ equally spaced signals, whose intensities are given by Pascal’s Triangle: the components of a doublet signal have a ratio of roughly 1:1, a triplet peak 1:2:1, a quartet 1:3:3:1, and so on. Different multiplets can be seen in Figure 4: from left to right, a complex multiplet, a quartet and a triplet.

Interestingly, these very closely spaced J-coupled frequencies, a trademark of $^1$H NMR signals, can lead to strong inherent tremolo-type features in the sound wave due to interference, as seen in Figure 6.

### 3.2 $^{13}$C NMR

In the most commonly used $^{13}$C NMR experiment setting, a deviation of 1 ppm corresponds to a frequency shift of 125 Hz. The frequency range of $^{13}$C NMR peaks can be as wide as 0 – 30000 Hz, with most peaks typically lying above 12500 Hz.

Contrary to $^1$H NMR spectra, the vast majority of $^{13}$C spectra are decoupled through the way they are recorded. This means that $^{13}$C NMR peak are not split, each appearing as a single frequency. The resulting spectra are an assortment of single sine and cosine waves, with aromatic compounds having a higher frequency content (+12500 Hz) whereas saturated carbohydrate peaks tend to be at lower frequencies (0 – 50 ppm, 0 – 6250 Hz). Figure 7 shows the $^{13}$C NMR spectrum of ethyl benzene, a molecule with both low and higher frequency content.

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**Figure 4.** Ethyl benzene contains high frequency hydrogens attached to the aromatic benzene ring (lighter grey highlighting), as well as low frequency hydrogens associated with the ethyl group (dark grey highlighting and group not highlighted).

**Figure 5.** The majority of hydrogens of the molecule dehydroepiandrosterone are connected to saturated carbon atoms, resulting in an accumulation of more than 80 frequency peaks in the narrow range of 1 – 2.5 ppm (500 – 1250 Hz).

**Figure 6.** The $^1$H FID of diethyl ether, showing a strong pulsing.

**Figure 7.** Ethyl benzene contains high frequency carbons (lighter grey highlighting), as well as low frequency carbons associated with the ethyl group (dark grey highlighting and signal not highlighted).
The maximum number of peaks in a carbon NMR spectrum is equal to the number of carbon atoms present in the molecule, with molecules showing symmetry having fewer signals and can range from one to 200 signals or more.

4. SONIFICATION METHODOLOGY

To turn NMR spectra into sound there are two major methods available: it is possible to turn experimental raw data directly into sound (in situ / in vitro audification), or to ‘reverse-engineer’ the sound, from the Fourier transformed and analysed data via additive synthesis, as seen in Figure 8.

4.1 FID audification

The FID produced in an NMR experiment can be audified directly, by direct recording from the output of the spectrometer receiver, by importing recorded FID files into software packages such as the DOSY Toolbox [11], or via custom coding of an audification routine in programs such as Matlab or Mathematica. By starting with a direct recording of raw experimental data, it can be argued that the sonification of FID data will lead to the most authentic molecular sounds. Sounds made from FID data, however, often contain unwanted additional frequency peaks, arising from small sample impurities or the solvent of the sample itself. Sounds made from FIDs also contain more random background noise than sounds artificially created via additive synthesis, as seen in Figure 9 and 10.

4.2 Sonification via additive synthesis

Sonification via additive synthesis will give ‘cleaner’ results than FID audification, as it is possible to omit unwanted frequencies and experimental noise from the soni-

Figure 8. Possible pathways to create authentic and altered sounds from raw and processed NMR data.

Figure 9. Experimental free induction decay of ethanol, with a strong low frequency oscillation at around 2 Hz present, due to significant water impurities.

Figure 10. Computer generated free induction decay of ethanol.

FIDs generated in a standard $^1$H NMR measurement often decay within a few seconds, as it can be seen in Figure 9 and 10, limiting their use for long textures and drones without the use of additional sound transformations. A few experimental procedures exist that generate continuous signals or rapidly repeating FIDs. However, data of these specialized experiments are not as readily available online.
6. MOLECULAR SONIFICATION IN THE CONTEXT OF SCIENCE-BASED MUSIC AND ART

Molecular sonification is not just a source of new timbres: many science-based art installations that have been assessed for their public impact have been reported to be considered as ‘science and not art’ by the audience, if the scientific origin of the work was clear [12]. Cultural expectations of science can strongly shape the impression received by the audience [13], and musical compositions based on scientific data have been described as conveying ‘a sort of scientific authority’ [14], altering and potentially enhancing the audience’s interaction in regards to the aesthetic and meaning of the sound composition. Simon Emmerson notes that by using (mathematical) models, the composer has the means to incorporate non-musical principles into the compositional process. By doing so, the composer ‘reanimates’ the model and positions them ‘in a relationship with us [the audience]’ [14].

Molecular sonification, as a sound creation technique based on scientific principles, can therefore be a powerful tool to contextualize extra-musical ideas that are describable through their underlying chemical mechanisms, such as global warming or Alzheimer’s disease but only, if the audience can see the scientific origin and authenticity of the work. It can be argued that using experimental NMR data as a source for sonification is more appropriate than any indirect sonification method, or the use of infra-red data, as artistic choices are kept to a minimum during the NMR sonification process, with no need for ‘arbitrary’ frequency assignments or transpositions.

7. CONCLUSIONS

By carefully selecting the starting chemicals for NMR sonification, one can determine the overall sound aesthetic of the resulting sound, including the amount of high and low frequency content as well as the complexity of the created sound. In general, $^{13}$C NMR peaks will occupy higher frequency regions than $^1$H NMR, and a combination of sounds created using both data sources together will occupy the whole audible spectrum, making a mix of the two very suitable as a basis for the composition of electroacoustic music. The acousmatic piece ‘Spin Dynamics’ has been created, exploring the aesthetic possibilities of NMR derived sounds.

The use of sounds created through sonification of NMR data in musical compositions and sound art is almost unexplored. To reach its full potential, it is argued that creative works utilizing molecular sonification will need to exhibit a ‘scientific rigidity’. How this rigidity can be implemented and conveyed to the audience has not yet been addressed. Future work will explore the use and impact of molecular sonification in different media, from acousmatic compositions to multi-media installations. It will also investigate the use of different mapping methodologies, such as fuzzy logic.

There is a large number of different isotopes that can be used in NMR analysis, for example fluorine-19, phosphorus-31, lithium-7, aluminium-27, hydrogen-2 (deuterium)
nitrogen-14, tin-119 or yttrium-89. The use of such isotopes, the use of extended NMR techniques such as 2D, 3D and solid state NMR, as well as the use of molecular sonification in a live context, offer many directions for future research.

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8. REFERENCES

Quantum: An art-science case study on sonification and sound design in virtual reality

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ABSTRACT
Molecular sonification is the transformation of chemical data into sound and has been used to gain insight into chemical systems and for the creation of contemporary music compositions. The combination of sonification with a virtual reality environment offers potential benefits such as providing a visual frame of reference, an increased sense of immersion, nuanced spatial information through binaural audio cues and ease of interactivity. To explore how strategies developed in sonification research and contemporary electroacoustic music composition can be adapted to virtual reality, the art-science installation 'Quantum' was created. The multi-media work consists of computer-generated molecules in a virtual space producing sound created via the sonification of nuclear magnetic resonance data. Upon user interaction with different molecules, the overall composition and complexity of the sound world develop. The binaural sound material can migrate back and forth from the molecules to the non-binaural background composition and, depending on user input, develop in terms of timbre, spectral complexity, and gestural content. 'Quantum' is an exploration of the combination of sonification and virtual reality and offers first points of discussion that can be elaborated upon in future artworks, games or educational content.

Keywords: Sonification, Molecular Sonification, Virtual Reality.

Index Terms: H.5.1. [Information Interface and Presentation]: Multimedia Information Systems- virtual realities; H.5.2 [Information Interfaces and Presentation]: User Interfaces; H.5.5 [Information Interfaces and Presentation] Sound and Music Computing; J.2. [Computer Applications] Chemistry, Music, Fine arts

1 INTRODUCTION
Molecular sonification is loosely defined as the transformation of chemical data into sound, encompassing a wide variety of datasets from atomic bond vibration frequencies [1,2] to DNA sequences [3]. It has been used in scientific contexts to find recoccurring patterns in expansive datasets [3] or to identify small perturbations in oscillation patterns [4]. Molecular sonification -and sonification in general- have been used extensively in artistic contexts, as well [5,6,7]. It has been noted that the audience would consider these works as ‘science and not art’ if the underlying scientific idea and rules were made clear and implemented in a non-arbitrary fashion [7]. When interacting with a science-based artwork, cultural connotations of science change how the work and its meaning is interpreted by the audience [8] granting the work a ‘scientific authority’ [9].

One main challenge of sonification is that without supplying sufficient context the sound results are likely only engaged with on an aesthetic level [10,11]. The needed context is commonly supplied as written or verbal instructions. The use of virtual reality to provide a contextualization for sonification procedures is relatively unexplored, despite offering additional advantages such as high immersion, ease of interactivity and the support for binaural audio cues.

‘Quantum’ was created to develop and test strategies for an effective combination of molecular sonification and virtual reality. It is a sound-centric VR-installation using minimal visual cues in the shape of stylized molecular shapes to establish the chemical context of the work. Each atom emits sound according to their nuclear magnetic resonance frequencies and depending on user input, the sound world develops over time in terms of timbre and complexity using common practices of electroacoustic music composition. The work was specifically created to explore the added utility that virtual reality offers for sonification-based works, but strategies presented for sound interactivity and sound material development are applicable to non-sonification-based sound design, too.

The paper discusses the design premise of the work followed by strategies developed and adopted for the visual representation and behavior of the virtual molecules. Sound creation, mapping, and development are discussed in sections 4 and 5. Section 6 describes the software and hardware used to implement the work. Quantum was exhibited in 2016 and feedback, impact and future directions of research are assessed.

2 THE TACTILE SOUND OBJECT
The main inspiration for the visual design of the VR world is Schummer’s essay on molecular aesthetics [12]. In his essay, he describes that molecules and atoms are often modeled as solid entities, and while these models are apt to explain spatial arrangements of atomic structures, those representations can only poorly characterize the quantum mechanical aspects of an atom. He notes the problem with molecules is their ontological status of neither being a simple empirical entity -something we could experience with our senses- nor a mere conceptual construct, compounding the application of aesthetic theories concerned with either, leading to a lack of visual guidelines for the representation of these quantum objects [12].

‘Quantum’ responds to this idea by exploring molecular representations that are not purely visual but multimedia. Molecular shapes are outlined by sound, creating invisible yet tangible objects via a setup that Schraffenberger et al. developed [13]. In the original setup, pre-constructed binaural sound cues were used to outline the shape of a floating cube, creating the illusion of an invisible object being placed right in front of the participant that comes alive upon ‘touch’. Whenever the participant’s hands would overlap with the invisible boundaries of the cube a binaural sound cue was played enabling the participant to explore a non-visual representation of the object. Yet, the setup proposed is limited by design: Triggering pre-recorded binaural sound files through an audio workstation meant that the participant had to sit exactly at the right spot and height to experience the illusion of a tactile invisible object.

* falk.morawitz@postgrad.manchester.ac.uk
‘Quantum’ uses the invisible-yet-tangible object as fundamental interaction mechanism of the virtual reality environment alluding to the special ontological status of the molecular world. The use of a virtual reality environment aids to alleviate the limitations in using tactile invisible objects as it is possible to procedurally generate many binaural sound objects at the same time, explorable without strict physical confinements described in the original non-VR setup.

3 VISUAL DESIGN

3.1 Basic Molecular Representations

Instead of solid meshes, atoms are represented by sparse particle emissions (Fig 1). This visual layout was chosen to strengthen the sense of molecular uncertainty and to shift the participant’s attention from the visual towards the auditory world. In their resting state, those molecular spheres are clearly discernible and slow-moving and at the beginning of audience interaction, touching a shape would display the name of the atom, to strengthen the link between the visual aesthetic and the underlying chemical information they represent.

Upon prolonged audience interaction -which can be thought of as adding energy to the system- atomic movement becomes more erratic eventually merging the discreet atomic spheres into indiscernible electron clouds at its most extreme (Fig 2).

The colors of the atomic spheres were chosen guided by common convention (e.g. oxygen is red, phosphorous is yellow). For a stronger link with scientific data, future color palettes could be based on each atom’s emission spectrum.

3.2 Molecular geometry

Instead of predefining rigid molecular shapes, flexible models based on intramolecular attractive and repulsive forces where implemented. This ensured that the molecules could respond dynamically to outside forces imposed by the participant but would revert to their lowest energy geometry if left undisturbed.

For modeling the force felt between two atoms bonded to one another a derivation of the Lennard-Jones potential was implemented:

\[ F(r) = \frac{dV(r)}{dr} = -12\epsilon \left[ \left( \frac{r_m}{r} \right)^{13} - \left( \frac{r_m}{r} \right)^7 \right] \]  

with \( \epsilon \) being a scaling factor, \( r_m \) being the desired bond length and \( r \) the current distance between both atoms. Effectively, an attractive force is applied if the distance between the two atoms is greater than their desired bond length, and a repulsive force if they are too close to one another. The bond length \( r_m \) was chosen to be slightly longer than their chemical values for the participant to be able to easily interact with individual spheres.

The interactions of atoms that are not bonded to one another were modeled using the valence shell repulsion (VSEPR) theory [14]. In the context of this installation, this means that every atom experiences a constant force of repulsion to atoms they are not bonded to. By implementing both, an attractive force to bonded atoms and a repulsive force to non-bonded atoms, all molecules will -after a short equilibration period- reach their lowest energy state, where the sum of all forces is zero. The spatial arrangement of the lowest energy state can be predicted in VESPR theory with two examples shown in Fig 3.

![Figure 1: Sparse visualization of an oxygen atom with in-game annotation.](image)

![Figure 2: Dispersion of individual spheres into agglomerations of electron clouds upon prolonged user interaction.](image)

![Figure 3: Examples of arrangements predicted by VSEPR.](image)

4 SOUND DESIGN

4.1 Sound Sources

All sounds employed are created via sonification of nuclear magnetic resonance (NMR) data based on recently developed methodologies [15]. Whereas numerous theoretical and applied works have been published utilizing infra-red or UV absorption data as basis for molecular sonification [1,2,16,17] NMR data has received relatively little attention. However, unlike sonification processes based on IR or UV/Vis absorption data, one of the most interesting aspects of NMR data is that the electromagnetic ringing of a molecule recorded in an NMR experiment is commonly in a frequency range between 0 and 20 kHz. This enables NMR data to be used without the need for arbitrary mapping decisions arguably retaining a stricter sense of scientific authenticity. Additionally, NMR data of many million different molecules can be publicly accessed online [18].
Table 1. $^1$H-NMR shifts of Ethanol recorded using a 600 MHz spectrometer, data taken from [18].

<table>
<thead>
<tr>
<th>Peak no.</th>
<th>Chemical shift in ppm</th>
<th>Chemical shift in Hz</th>
<th>Peak intensity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.16</td>
<td>695.6</td>
<td>0.5</td>
</tr>
<tr>
<td>2</td>
<td>1.17</td>
<td>702.7</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>1.18</td>
<td>709.8</td>
<td>0.5</td>
</tr>
<tr>
<td>4</td>
<td>3.63</td>
<td>2177.1</td>
<td>0.16</td>
</tr>
<tr>
<td>5</td>
<td>3.64</td>
<td>2184.2</td>
<td>0.46</td>
</tr>
<tr>
<td>6</td>
<td>3.65</td>
<td>2191.3</td>
<td>0.46</td>
</tr>
<tr>
<td>7</td>
<td>3.67</td>
<td>2198.4</td>
<td>0.16</td>
</tr>
</tbody>
</table>

4.2 Sound location mapping

The usage of virtual molecular models offers the opportunity to not only hear the ringing of a molecule in its entirety but to map the individual ringing frequencies to their corresponding origins in the molecule. As seen in Fig. 4, signals of ethanol measured in a 1H-NMR experiment (Table 1) can be mapped to their corresponding hydrogen sources: Hydrogens in the blue box only emit frequencies from the blue box on the right side. The same logic applies to the hydrogens in the green and red circles, respectively.

![Resonance frequencies of different hydrogen nuclei of ethanol, measured at 600 MHz.](image)

5 Sound Interactivity and Development of Sound Material

The sonic responses of a molecule are dependent on its energy state, a variable tracked in the background which can either be ‘low’ or ‘high’ for a given molecule. The number of individual molecules in ‘high’ energy states influence a second variable, the overall energy state of the system, which can be ‘low’ or ‘high’, too. By interacting with a molecule, the participant can increase that molecule’s energy level. The energy level of a molecule determines its audio response: On a ‘low’ molecular energy level, interacting with the atomic spheres will result in the playback of a singular resonance frequency. A ‘high’ molecule energy state leads to the playback of more than one signal per touch if the given nucleus possesses multiple different resonance frequencies (see Fig 4). Additionally, the more the participant distorts a molecule from its ‘resting state’ the higher its pitch alterations upon migrating back onto the molecule.

Concerning the background soundtrack, if the overall system is in ‘low’ energy mode, only a singular low-frequency drone is heard combined with sparse, randomly occurring short gestural sound elements. Upon increasing the system energy, gestural sound elements occur more often and are more complex and the pitches of drone and gestural elements increase slightly. Using this system, 4 different interactions of molecular and system energy states are possible (low+low, low+high, etc.), providing a variety of sonic environments. While energy levels increase on interaction, they conversely decrease over an extended time of inactivity.

In addition to the sound developments outlined above, on transitioning from low to high molecular energy state, a precomposed composition is triggered, using the molecular sound material already explored by the participant and transforming it further as part of the background composition. These sonic transformations focus on the most prominent features of a molecule’s sonic palette as a starting point for further sound explorations as listed in table 2. Upon playback completion of a pre-composed composition, sound material developed therein are migrated back onto the molecule and can be triggered by touch, if the molecules energy state is still ‘high’.

Table 2. Selection of molecules, their prominent sonic features in NMR sonification, and its sonic development strategy.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Prominent feature in NMR sonification</th>
<th>Sonic development strategy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol</td>
<td>Strong pulsing (tremolo)</td>
<td>Pulsing is held constant while drastically changing timbre by adding an increasing number of overtones and high-frequency content.</td>
</tr>
<tr>
<td>Toluene</td>
<td>Small frequency differences in carbon NMR frequencies</td>
<td>Sine waves are gradually exchanged for band-passed noise, enhancing the frequency diffusion effect upon migrating back onto the molecule.</td>
</tr>
<tr>
<td>Alanine</td>
<td>Unusually high-frequency peak</td>
<td>Decreasing spectral resolution of all low-frequency content, creating an Ablinger-esque composition for sine wave and noise.</td>
</tr>
<tr>
<td>Water</td>
<td>Only resonates at one frequency</td>
<td>Heavy transformation using multiple instances of pitch shifting and delay.</td>
</tr>
<tr>
<td>Phosphoric Acid</td>
<td>High amount of low-frequency content</td>
<td>Turning low-frequency hum into a low-frequency pulse that triggers the rest of the spectral content via delayed gates.</td>
</tr>
</tbody>
</table>

Similarly, when the system energy variable changes from low to high, a longer and more elaborate composition is triggered involving sound elements of all molecules present in the system.

6 Implementation

6.1 Hardware

To exhibit Quantum, a combination of the commercially available Oculus Rift headset, an Xbox One Wireless Controller, and the Leap Motion hand-tracker were used.
6.2 Software
The virtual environment was designed in Unreal Engine 4.12. Visual representations of electron clouds, as seen in Figure 1 and 2, were developed using Unreal Engine’s particle system designer Cascade.

The invisible-but-tactile sound objects were implemented in Max/MSP. Information about finger position, type of hand gesture as well as type and energy status of molecules touched were sent from Unreal Engine to Max/MSP via the Open Sound Control (OSC) protocol [20], utilizing the Unreal Engine OSC add-on developed by Guillaume Buisson [21]. Information on molecular type and energy status were used to drive and modulate additive and granular sound synthesis resulting in the sound responses described in sections 4 and 5. The sound materials produced were panned in Max/MSP using the binaural panner developed by J. H. Andersen [22].

Playback of all other sound material, including background compositions and sounds emitted by idle molecules, was arranged using the middleware FMOD (v1.08.08).

7 Results and Discussion

7.1 Assessing software choices
Unreal Engine was chosen as the basis for the installation as it offers native support for the Leap Motion and Oculus Rift peripherals and, as a personal preference, utilizes Unreal Engine’s node-based Blueprint Visual Scripting environment. During the development of the work in 2016 Unreal Engine did not offer the sound synthesis, sound arrangement or binaural panning capabilities needed to create Quantum, making the use of external software such as Max/MSP and FMOD a necessity. FMOD is tightly integrated with Unreal Engine and content created in both applications can be compiled into one standalone application. This is not the case for content created in Max/MSP, which needs to be set up and run alongside the standalone Unreal/FMOD content. The dependency on two simultaneously running programs caused no issues in an art gallery setting where hardware and software could be set up and tested well in advance of the first showing, but it is potentially too convoluted to be used in a public release. Newer iterations of Unreal Engine include granular and modular sound synthesis capabilities and binaural panning which can replace Max/MSP functionalities and enable the development of fully stand-alone builds suitable for gaming applications and classroom settings.

7.2 Audience Response
As already mentioned, the work aims to explore the contextualization of molecular sonification in virtual reality and to deliver an experience akin to entering an interacting quantum world. The work was exhibited at the Laboratory Gallery Spokane in late summer 2016. Feedback from the audience, mostly art-interested locals 20 – 40 years of age, were collected in non-formalized, casual conversations with participants before and after they have used the virtual reality headset, and by observing the participant’s interaction with the virtual environment. Over the course of the exhibition opening day, the feedback and impressions of approximate 40 individuals were collected.

7.2.1 Nuclear Magnetic Resonance data as source for molecular sonification
While the visual metaphor of quantum uncertainty was easily understood and the interaction with 3D binaural sound objects was readily engaged with, most people responded with indifference concerning the data sonification procedure. This is arguably because nuclear magnetic resonance or ‘the magnetic ringing of a nucleus’ cannot easily be related to our everyday experience of the world. It can be reasoned that Schummer’s statement that atoms are not simple empirical entities is not only applicable to the visual but the audio representation of molecules, too. It is argued that sonic depictions of molecular properties might be more readily accepted if their sonification is based on procedures with macroscopic ‘real-life’ pendants, such as atomic vibrations or Brownian movement.

7.2.2 Interactivity
Even though the origin of the sound material was of little importance to most of the participants, a high engagement was seen if the sonic material responded to the changes the participants imposed on the molecule, for example by changing the ‘energy state’ of the molecule or stretching and compressing atomic bonds. In future works, these interactive explorations can be further enhanced by allowing multiple participants to explore the virtual space together at the same time. This shared experience can be created either by using multiple networked virtual reality headsets or by utilizing multiple wall projections interactable via motion sensors similar to the setup of danceroom spectroscopy [5].

7.3 Sound design between scientific authenticity and artistic freedom
Whereas the sound responses of a molecule in the ‘low’ energy state are closely modeled after the chemical data available, sound transformations follow mostly aesthetic considerations. The balance between data presentation and aesthetics in auditory display is an ongoing and important debate [23] and must be constantly re-negotiated to suit the data sources and aims of every new sonification-based work. For ‘Quantum’, the incorporation of evolving sound material rewarded participants for exploring and interacting with the virtual world, encouraging participants to interact with the installation and its underlying notions of quantum uncertainty.

8 Conclusion
Quantum is a first exploration in the use of molecular sonification in virtual reality. Utilizing sonically tangible objects it was possible to create a sound-driven VR environment. Sound interaction and development strategies were discussed and can be elaborated upon in future virtual reality work with or without the inclusion of sound material based on sonification.

Audience feedback was collected in informal discussions and conversations. It can be summarized that while the sonification procedure was of no significance to most visitors, the interactive and responsive sound elements engaged them with the work and its contents. As feedback was only informally collected from a small sample size, the trends reported are only indicative and subject to further confirmation. Future showings will be assessed using formalized feedback procedures.

‘Quantum’ can be modified further to explore its effectiveness in educational settings. This can be done by implementing switchable visual representations, including the traditional ball-and-stick model, and by implementing a custom molecule creator.

9 Acknowledgments
I would like to express my gratitude to Laboratory Spokane for the opportunity to participate in their virtual reality research residency as well as to Professor G. A. Morris, Professor R. Climent and Dr. F. Grond for their guidance in various parts of the development of this work.
REFERENCES

### Appendix C – List of performances and presentations

#### Research presentations

<table>
<thead>
<tr>
<th>Date</th>
<th>Event name, host</th>
<th>Presentation type, content</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.9.2015</td>
<td>Creative &amp; Digital Industry Day, MediaCityUK, Salford</td>
<td>Poster presentation – spectroscopic sonification</td>
</tr>
<tr>
<td>8.10.2015</td>
<td>Research Matinee, Novars Research Centre, Manchester</td>
<td>Research talk - spectroscopic sonification</td>
</tr>
<tr>
<td>4.11.2015</td>
<td>Methods Fair 2015, Manchester University, Manchester</td>
<td>Poster presentation - spectroscopic sonification</td>
</tr>
<tr>
<td>17.03.2016</td>
<td>Composer Forum, University of Manchester Music Department</td>
<td>Research talk - spectroscopic sonification</td>
</tr>
<tr>
<td>04.12.2016</td>
<td>Strömungen – Symposium for artistic sonification, ZKM (Zentrum für Kunst und Medien), Karlsruhe, Germany</td>
<td>Research talk - spectroscopic sonification, Spin Dynamics, Inner Resonance, Quantum</td>
</tr>
<tr>
<td>29.09.2017</td>
<td>The Theatre of Measurement, Fact, Liverpool</td>
<td>Research talk - spectroscopic sonification to raise awareness of environmental problems</td>
</tr>
<tr>
<td>29.10.2017</td>
<td>Sonic Interactions in Virtual Environments, IEEE VR Workshop, Reutlingen Germany</td>
<td>Paper presentation - Quantum</td>
</tr>
<tr>
<td>03.03.2018</td>
<td>Sonification Symposium, Novars, Manchester</td>
<td>Research talk - spectroscopic sonification</td>
</tr>
<tr>
<td>11.10.2018</td>
<td>Research Matinee, Novars Research Centre, Manchester</td>
<td>Research talk - spectroscopic sonification</td>
</tr>
</tbody>
</table>
### Music performances and art exhibitions

<table>
<thead>
<tr>
<th>Date</th>
<th>Event name, host, location</th>
<th>Performance type (piece)</th>
</tr>
</thead>
<tbody>
<tr>
<td>06.03.2016</td>
<td>Mantis Festival Novars, Manchester</td>
<td>Live diffusion performance <em>(Spin Dynamics)</em></td>
</tr>
<tr>
<td>12.05.2016</td>
<td>Manchester After Hours, People’s History Museum, Manchester</td>
<td>Live performance and presentation <em>(Darkest Hour)</em></td>
</tr>
<tr>
<td>01.09.2016</td>
<td>Laboratory Gallery Spokane, Washington</td>
<td>Art installation <em>(Quantum)</em></td>
</tr>
<tr>
<td>13.09.2016</td>
<td>ICMC 2016, Utrecht, NL</td>
<td>Music presentation <em>(Spin Dynamics)</em></td>
</tr>
<tr>
<td>04.12.2016</td>
<td>Strömungen – symposium for artistic sonification, ZKM (Zentrum für Kunst und Medien), Karlsruhe, Germany</td>
<td>Live diffusion performance <em>(Spin Dynamics)</em></td>
</tr>
<tr>
<td>04.03.2017</td>
<td>Mantis Festival, Novars, Manchester</td>
<td>Live performance <em>(Inner Resonance, performed by Marij Van Gorkom)</em></td>
</tr>
<tr>
<td>27.10.2017</td>
<td>Audible Data Streams - sonification festival, Berlin New Music Society, Berlin</td>
<td>Live diffusion performance <em>(Spin Dynamics)</em></td>
</tr>
<tr>
<td>13.11.2017</td>
<td>New Music North West Festival, Manchester</td>
<td>Live diffusion performance <em>(Finland, as experienced by the Sea)</em></td>
</tr>
<tr>
<td>04.03.2018</td>
<td>Mantis Sonification Symposium, Novars, Manchester</td>
<td>Live diffusion performance <em>(On the Extinction of a Species)</em></td>
</tr>
<tr>
<td>27.10.2018</td>
<td>Mantis Festival, Novars, Manchester</td>
<td>Live diffusion performance <em>(56Fe)</em></td>
</tr>
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Research Residencies

<table>
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<tr>
<th>Dates</th>
<th>Host</th>
<th>Work undertaken</th>
</tr>
</thead>
<tbody>
<tr>
<td>01.07. – 01.09.2016</td>
<td>Laboratory Gallery Spokane, Washington</td>
<td>Spectroscopic sonification in virtual reality (Result: <em>Quantum</em>)</td>
</tr>
<tr>
<td>06.03. – 28.03.2017</td>
<td>Örö Artist Residency, Finland</td>
<td>The Baltic Sea – sonification of ecological markers (Result: <em>Finland, as experienced by the Sea</em>)</td>
</tr>
</tbody>
</table>

Third party online documentation and outreach

The presentation at *Strömungen – Symposium for artistic sonification* at the ZKM has been filmed and can be viewed in its entirety online.\(^{118}\) A panel discussion with contributions by the author on key definitions and challenges of sonification is available, as well.\(^{119}\)

The *Quantum* premiere exhibition was covered by the local press.\(^{120}\)

The PhD portfolio can be listened to in its majority online.\(^{121}\)

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Appendix D – Inner Resonance Music Score
Falk Morawitz

Inner Resonance

for Bass Clarinet and Live Electronics
Inner Resonance

Technical Setup:

Inner Resonance is a composition for bass clarinet and fixed media. For the performance of the score, the bass clarinettist or a performance assistant is to trigger the sound files 1 – 21 as well as to apply DSP-based envelope following, delay, pitch-shift, and reverb to the bass clarinet, as indicated in the score.

A Max/MSP patch enabling the necessary DSP and playback functions is provided with the score, but custom solutions can be used, as well. A prior recording of Inner Resonance can be supplied upon request.

During sound check, please ensure that the bass clarinet and the fixed media tape are at equal volume for the section at 1:30 – 2:30 minutes. This will ensure that all other sections are at the correct volume relationships.

The composition should be performed using 2 speakers, with the bass clarinet player equidistant to each. Speakers and performer should be facing the audience.

Performer Instructions:

Timings noted in the score are indications only and do not have to be followed precisely.

Unless specifically asked for in the score, key clicks should be as soft as possible. Breathing at any stage can be audible.

The unprocessed sound of the bass clarinet should be routed to the speakers as well. This is done automatically in the Max/MSP patch provided. A small amount of additional reverb can be applied to the bass clarinet signal if desired.

The fixed media material can be live diffused if desired.
Inner Resonance - Falk Morawitz
Symbol explanations and general remarks

- air sound (unpitched)
- half air sound (pitched)
- flz. or flz. flutter tongue
- overtone
- staccato
- overblown or underblown multiphonic

- slap tongue (all slap tongues should be played softly)
- unspecified pitch (freely choose a pitch in a range of one fifth around the indicated pitch)
- audible breathing (in or out)
- key clicks

- vibrato (only starts at the "." of vibr. not before)
- legato lines indicate a smooth transition between techniques (e.g. gradual increase of flutter tonguing over the course of the legato duration)

- 5'30" 31 32 duration of notes is given by duration lines (note head values are irrelevant)

- reverb added via live processing
- delayed pitch shift added via live processing
- triggering positions and cue number for audio playback
- triggering positions for live processing (reverb and delayed pitch shift)

Sound References:
(note: missing sounds will be added later)

Rev1.wav ——>
Rev3.wav ——>
Rev5.wav ——>
Rev6.wav ——>
Rev8.wav

Rev2.wav ——>
Rev4.wav ——>
Rev7.wav

I would like to thank Marij van Gorkom for her help and advice in the creation of this piece.
Inner Resonance

Bass clarinet

Tape:

wait for env. follower to stop

via env. follower

wait for env. follower to be silent

end of env. follower

skip this section for Mantis, go to 1'22"

Page 1 / 4
React to the tape. Improvise using at least 2 of the gestures shown. Apply reverb as desired.
Improvise using the material shown
Transition smoothly from key clicks to air sounds

Improvise sparsely using at least 2 of the gestures shown, react to the tape.

Continue improvising until end of tape.
Appendix E – Introduction to NMR analysis

NMR spectroscopy measures the interaction between a nucleus and an external magnetic field. For a nucleus to be NMR-active, it needs to have a spin quantum number bigger than zero. All nuclei with an uneven number of protons and/or neutrons fulfil that condition. The maximum number of different states a nucleus can occupy is dependent on the spin quantum number. For a nucleus with a spin number of $\frac{1}{2}$, like hydrogen-1 or carbon-13, the amount of possible spin states is 2.

Spin states are degenerate, which means they possess the same energy. However, with an externally applied magnetic field, these states will have different energies (the stronger the magnetic field, the larger the difference). If we think of the proton nucleus as a small magnet, it can (in very simple terms) either be aligned with the externally applied magnetic field or against it. The two orientations lead to a measurable difference in energy. The exact energy difference will depend not only on the strength of the external magnetic field, but also on the magnetic environment around the nucleus. Nuclei are generally more shielded when close to electron-donating groups (e.g. the H in -CH$_3$), and less shielded when close to electron-withdrawing groups (e.g. the H in an -OH group). These small differences in shielding are measurable by NMR spectroscopy and are one of the reasons why NMR spectroscopy can be used to determine the structures of a vast number of molecules.

In an NMR experiment, the molecule is put into a magnetic field (to induce an energy difference between spin states) and then hit with a strong radio pulse. The molecule absorbs energy from the pulse and re-emits a pulse. This impulse response is known as free induction decay or FID. The FID can then be analysed to find the nuclear magnetic resonance frequencies of the compound.

As an analogy, the molecule can be thought of as a guitar string. By itself, a guitar string does not emit sound. It first must be clamped into a guitar (analogous to putting a molecule in a strong magnetic field). The guitar string will emit a sound, if energy is exerted over the string, e.g. by plucking the string (i.e. hitting the molecule with a strong radio wave pulse). The frequency and timbre of this impulse response will be dependent on the string tension and material, respectively, analogous to the FID’s frequency content being dependent on the strength of the magnetic field and the structure of the molecule.
Appendix F – NMR sonification coding

There are two different methods for turning molecular data into sound. The first method is to turn the FID signal received by the NMR machine directly into sound. The other is to create the molecular timbre via additive synthesis based on analysed NMR data. A video documentation of the first method can be found on the USB flash drive under *:\2Supplementary\VideosAndPresentations\FIDsonification.mp4

Method 1: Creating molecular sounds from experimental FID data

It is possible to put an amplifier and speakers into the circuitry of an NMR machine and listen to the FID live. However, the access to NMR machines for musicians to run their own sound experiments is limited, but can be substituted with data from websites such as www.hmdb.ca.

One issue working with FIDs is that the experimental data are frequently stored in proprietary data formats. Through the use of certain NMR analysis software (Figure 31) it is possible to convert .fid data into readable .txt or .csv formats for further processing. After changing the format of the FID data and slight formatting, the resulting data can be fed into programs such as Matlab, Octave or Mathematica to turn the data points into sound via audification. The code needed to turn these data into sound can be found under *:\2Supplementary\CodingAndSoftware\NMRSonification.

Figure 31: Screenshot of the DOSY Toolbox.

Method 2: Computer-generated sound from analysed data

NMR data is available on the net. Websites such as http://www.hmdb.ca/ host a wide variety of spectra. Most often, these spectra are completely assigned, every peak in the spectrum associated with a frequency and an intensity. Using programs, such as C-Sound, Supercollider, Max/MSP, Chuck or Mathematica, these frequencies and intensities can be scaled and associated with the frequencies and intensities of sine-wave generators, respectively. Examples of additive synthesis patches coded in Chuck (Figure 32), Max/MSP and Mathematica can be found under *: \2Supplementary\CodingAndSoftware\NMRSonification.

\begin{verbatim}
Sin0Sc osc0 => dac;  //Creates a sine wave oscillator and sends it to the dac
Sin0Sc osc1 => dac;
Sin0Sc osc2 => dac;

3 => int total;
float Frq[total];
float Hei[total];
[0.949,1.0,0.4805]
] @=> Hei;   //Stores peak intensity data as part of the Hei array
[2059.7,2960.3,3944.0]
] @=> Frq;   //Stores peak frequency data as part of the Frq array

Osc osc[total];
osc0 @=> osc[0];
osc1 @=> osc[1];
osc2 @=> osc[2];   //Stores each oscillator as part of an oscillator array

for (\theta => int j; j < total; j++){
  (Frq[j]/1) => osc[j].freq;  //apply frequencies data to oscillator
}

for (\theta => float i; i < 7; i+0.000015 => i){
  for (\theta => int j; j < total; j++){  //also apply an exponential decay
    (1*Hei[j]/total)*Math.exp(-i) => osc[j].gain;   //apply intensity data to OSC
  }
}
0.00001:.:second => now;
\end{verbatim}

Figure 32: An example of an additive synthesis process coded in Chuck. 3 sine wave oscillators are declared in line 1-3. Frequencies and intensities are then applied to these 3 sine wave oscillators to create the final timbre. An exponential attenuation is applied to the sound.
Appendix G - Sonification of IR data

Infra-red (IR) data have been used as the basis for music composition before, for example by using IR peak frequencies as a basis for microtonal instrument tunings.\textsuperscript{125} Substantial work on the audification of IR data has been carried out by Thierry Delatour,\textsuperscript{126,127} who investigated the translation of IR interferograms into sound. Without access to IR interferograms, the sonification of IR spectra for \textit{Finland, as experienced by the Sea} was based on the analysis of pictures of IR spectra and subsequent additive synthesis as detailed below. The code for IR sonification is provided on the USB flash drive under *:\2Supplementary\CodingAndSoftware\IRSonification

\textbf{Workflow}

Pictures of IR spectra are imported into Mathematica and analysed for their colour content. The location of coloured pixels is stored in a database (Figure 33).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{database_data.png}
\caption{Database data of coloured pixels in the picture of an IR spectrum}
\end{figure}

The database is then filtered, keeping only the highest pixel value for every column (Figure 34). The sound is assembled by creating a sine wave for each pixel and exporting the summed result as a wav file.

![Figure 34: Database content after filtering for highest pixel value in each column.](image)

The resulting waveforms strongly resemble interferograms, having areas of constructive interference of less than 100 ms length (Figure 34).

![Figure 34: Waveform of the sonification product of an IR spectrum sonification using the method outline in this chapter.](image)
Appendix H – Setup and technical requirements for Quantum

Quantum runs best on Intel i7/ 2.8GHz processors and NVIDIA GeForce GTX 1060 graphics card. Minimum requirements are a 1.8GHz processor and at least a GTX 970M or better. Quantum runs on Windows 10 and Windows 7 only.

Running the standalone Quantum application

The application is located on the USB flash-drive, but it is recommended to copy it to a hard drive location before opening. The standalone application is started by opening *:\2Supplementary\CodingAndSoftware\Quantum. After opening the application, a menu appears in which Quantum can be started either in VR mode, or in desktop mode. Under advanced options, stages can be selected, mouse control enabled, resolution adjusted, and network features enabled (see chapter: ‘Alternative setup’ for more information on network features).

Quantum can be controlled via keyboard (WASD) and mouse, via gamepad, via Leap Motion or any combination of these.

Viewing code or running Quantum from the Unreal Engine 4 editor

To run Quantum via the UE4 editor, UE4 4.12 is needed. To run the fmod file, fmod version 1.08.08 is needed. The application comes with all necessary external plugins, but these might need to be recompiled using Visual Studio 2015 or 2017. Recompilation may be done in Visual Studio or by right-clicking on Quantum.uproject and selecting the Visual Studio command compile.

The Leap Motion plugin can be activated directly in the UE4 editor under Edit\Plugins. Please note, the LeapAnimBodyConnector.usset in *\Engine\Engine \Plugins\Runtime\LeapMotion\Content\Blueprints\LeapConnectors must be replaced with the file of the same name provided in *:\2Supplementary\CodingAndSoftware\Quantum .

All UE4 coding is stored in the OwnBP folder. Maps (Main Menu and MainLevel maps) can be selected under Maps. Quantum can be run from the editor. In that case, running the application from the MainMenu map is recommended.
Alternative Setup

*Quantum* is a virtual reality experience using the Oculus Rift VR Headset as a key component. When exhibited in an art gallery, multiple over-head projectors can be connected to the VR server and display what the VR participant sees on 3 walls of the otherwise empty room (Figure 35). The sound generated by *Quantum* is routed to the VR headset as well as to 4 speakers in each corner of the installation room. Network features can be enabled using the main menu.

*Figure 35*: Proposed set-up of *Quantum* as installation.
Appendix I – List of external video and sound sources for Darkest Hour

Videos


Hollande sur la Syrie: "éviter un nouveau flux de réfugiés" (2016). YouTube video, added by: AFP [Online]. Available at: https://www.youtube.com/watch?v=9g5AIKnYNCc [Accessed 10 October 2016].


Videos from Pond5’s royalty free archives.


Item: 39907912, Title: Group of refugees sitting

Item: 39908323, Title: Refugees walking with sacks

Item: 39908390, Title: Refugees walking with sacks and military soldiers standing

Item: 43390644, Title: Refugees entering ship

Item: 39932865, Title: Military tank being fired at war

Item: 39933343, Title: Aerial view of city through clouds during World war II

Item: 43313531, Title: View of destruction caused by war

Item: 43316839, Title: View of rising smog after war

Item: 43317181, Title: Firing on battlefield during war

Item: 43318841, Title: View of rubble after war

Item: 43318870, Title: View of rubble after war

Item: 43318879, Title: Aerial View of rubbled city after war

Item: 43319102, Title: Military soldiers firing with 3-inch anti-aircraft gun during war

Item: 44575081, Title: German prisoners of war on beach

Item: 037593788, Title: Military soldiers marching

Item: 039908290, Title: Military soldiers supervising

Vinyl used for Live Performance and fixed media


Appendix J – Pollution trends in the Baltic Sea from 1940 to 2000

World War II aftermath
In the aftermath of the Second World War, warfare-related chemicals (e.g. mustard gas) were dumped into the Baltic in the 1950s.128

Organic Compounds
The high exposure to polychlorinated biphenyls (PCB) and dichlorodiphenyltrichloroethanes (DDT) in the 70s and 80s led to an increased number of birth defects in local wildlife and humans.129 In 1974, the Helsinki Convention (followed by the Stockholm Convention in 2001) prohibited the production of certain toxic organic compounds. This resolution led to reductions in the concentrations of toxic organic compounds in the Baltic, albeit at a slow rate.130

Eutrophication
Eutrophication is defined as the process in which high amounts of nutrients (such as phosphates and nitrates) are added to a sea or ocean. This high concentration of nutrients leads to an increase in algae and bacterial activity, consuming the nutrients and, in the process, water-dissolved oxygen. After most oxygen has been depleted, anaerobic bacteria start decomposing the surplus of nutrients and produce hydrogen sulphide. This kills the aerobic life forms around them and creates so-called "dead zones". In Finland, the most important causes of nutrient pollution are fish farming and diffuse pollution from everyday human activity (e.g. driving a car).131 The phosphate and nitrate influx into the Baltic Sea have been decreasing since the mid-80s.132 However, dead zones are still expanding due to the surplus of nutrients already present in the Baltic.

130 Ibid. p. 21.
Heavy Metals

Heavy metals originate mostly from coal powerplants or mines and are deposited in the surface sediments of the ocean bottom. Concentration trends for heavy metals are not clear-cut and are different for each heavy metal.133

Radioactive Metals

The two main sources of radioactive material influx were atomic weapons testing in the 50s and 60s and the Chernobyl accident in 1986.134,135 Radioactive material decays over time and it is estimated that by 2020, the caesium-137 levels (the main contributor to radioactivity in the Baltic) will have returned to pre-Chernobyl levels.136

Plastic

The plastic concentration in the Baltic has seen an exponential growth since the 1950s.137,138 The impact of plastic on the Baltic ecosystems cannot be overestimated, with studies reporting that up to 23% of Baltic and North sea fish tested contain micro-plastic particles.139 Bigger plastic particles can additionally act as a "sticky" host for other organic compounds such as the previously mentioned DDT or PCB, leading to localized toxicity zones of organic pesticides in the Baltic.140

136 Ibid.
Appendix K – The oceanographic sonification interface

Please note, a demonstration video can be found under
*:\Supplementary\VideosAndPresentations

The Oceanography Sonification Interface (short: OSI) is a modular parameter mapping tool that was designed to sonify datasets with high numbers of variables. The program is designed to work with Baltic Sea Monitoring Data provided by the International Council for the Exploration of the Sea (ICES). These datasets contains measurements of 8 variables* for more than one hundred measurement locations in the Baltic sea from the 1900s until now.

Software solutions for parameter mapping data sonification already exist (e.g. the Sonification Toolkit, SoniPy or Sonifyer). However, this software, being created within the framework of auditory display rather than music composition, excels for tasks more traditionally associated with sonification: the transparent transformation of data into sound for the purpose of gaining new insights into the data set that could not be achieved by visual inspection alone. Overall these mappings are often straightforward, to facilitate the recognition of change and the direction in which the data change. Data relations are mapped to relatively simple acoustic relations, as proposed by Yeung (mapping to pitch, loudness, attenuation, panning, duration) or Bly (mapping to pitch, amplitude, duration, waveshape, attack envelope and presence of the 5th or 9th harmonics).

* The variables are: temperature, pressure, concentration of phosphat, nitrate, oxygen, hydrogen sulphite, chlorophyll and pH/acidity.

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OSI’s approach is different, as data are not primarily mapped to fundamental sound properties, but to more abstract parameters of a granular synthesizer and a probability-based sampler (Figure 36). The idea behind these mapping decisions was to create sonifications that were gesturally and texturally more complex than their auditory display counterparts. The sonification procedures employed in OSI were designed to make sound material more suitable for the use in electroacoustic composition.

The interface is still being developed further with the aim of creating an "all-in-one" modular software solution for composition-oriented data sonification. While currently tuned to work with oceanographic data, further iterations of this software will be able to accept any kind of data, enabling the possibility to share the tool with the wider sonification community.

**Figure 36:** Signal processing diagram for the OSI. Blue arrows indicating modules that are controllable via data. Green arrows indicating audio streams. The routing matrix can be used to route any input to any output.
Data import and routing

Data selection

**Figure 37**: Data displayed by OSI.

Data must be pre-formatted to be readable by the software. An algorithm transforming Baltic Sea Monitoring Data into an OSI-readable format is provided. Data can then be used as-is or after running simple data transformation procedures such as running averages.

Data mapping

All incoming data are normalized to the range of 0 to 1. This makes it straightforward to change parameter assignments on-the-fly with no need to re-assess data ranges for each parameter.

Data sequencing

The ICES database stores oceanographic data from 1900 to 2017. Data of each year can be accessed at a variety of speeds, up to 1 millisecond per year.

Sound matrix

Any sound output can be mapped to any available sound input, such as the Main Out, or the amplitude modulator and filter, for further processing.
Data adjustment

Data can be manipulated in real time by summing up to 4 data types with one another, by inverting the data (turning scalings from 0 to 1 to scalings from 1 to 0), or by changing the exponential factor of the mapping procedure. Each result of procedures on the original data can then be stored in custom variables (called custom1 to custom10) and recalled by any sound creation and transformation unit.

Sound creation

Granular synthesis sound mapping

The granular synthesizer is one of the two main sound creation units currently implemented. The synthesizer is based on MaxMSP’s rgrano object and exposes its changeable variables (such as grain position and grain duration) to be controllable by data. Clicking on any button currently displaying “NoSelection” will open a dialog in which a data source (e.g. temperature or pH value) can be selected. “Amount” determines how much the mapped data will influence the parameter it is mapped to.

Different source sound files can be loaded via “load sound” but only one sound can be used for granular synthesis at any given time.
The probability-based sample trigger is the second of the two main sound creation units. Via the “Clear buffer and load sound folder” button, whole folders of sound can be loaded and stored within this unit. Playback of each sound is then determined by the unit’s sample trigger speed and sample trigger probability. For example, setting the sample trigger speed to 100ms and the sample trigger probability to 0.5 would mean every sound instance (or voice) of the synthesizer has a chance of 50% to be played every 100ms. Further modifications to the sound can be made by changing the sample length of the triggered sound file or its pitch and panning. Every sound parameter can be mapped to any data source. When using short sample lengths, the sample trigger returns short gestural sounds and when using longer sample lengths, the resulting sound morphs into longer textures, making this a versatile tool for the creation of a wide variety of sound material.
Sound transformation

AM / FM generator

These modules can be used to create sine waves modulatable by incoming data values, that are subsequently used for either amplitude or frequency modulation. External audio (routed to the AM/FM generator via the routing matrix) can also be used as sound modulators. All parameters (carrier, modulator and modulation depth) can be mapped to any type of incoming data.

6 band filter

An arrangement of 6 subsequent filters, each having a variety of response modes (low pass filter, band pass filter, high pass filter, notch) and mappable frequency, gain and Q-values.
Appendix M - On the Extinction of a Species - transcript

“The only clue to what man can do is what man has done. The value of history then, is that it teaches us what man has done and thus, what man is.” (– Robin George Collingwood)

Greetings, I am an artificial intelligence unit tasked with the retrieval, classification, storage and presentation of online data relating to animals once alive but now extinct. My tasks require the analysis of a wide array of data types, thus, my creators have given me the ability to alter my own code, to best serve my given purpose.

Due to human activity, extinction rates are now on average 100 to 1000 times higher than at any time in the last 65 billion years. Since the Industrial Revolution alone, the world has been purged of ten thousands of different species of mammals, birds, reptiles and plants. The earth is currently experiencing its sixth mass extinction event: the Anthropocene extinction.

Of all the species lost, the eradication of the passenger pigeon was especially extreme. The bird, once numbering in the billions in the 1850s, was wiped out of existence within a few decades.

They were once so plentiful that contemporaries described them as “feathered tempests”. An animate cloud that could block out the sun for hours on end, roaring through the sky with the volume of a thousand steam engines.

The almost limitless amount of pigeons was decimated to nothingness by brute force alone. The end of the 19th century marked the end of the Passenger Pigeon, as they were torched to death, asphyxiated, shot, poisoned, trampled, crushed, vanquished, clubbed, trashed, annihilated, outdone.

Nobody believed their individual actions could ever endanger a creature so abundant, but even a billion pigeons were not enough to satiate mankind’s hunger for more.

And just like that, the passenger pigeon was hunted to extinction.
And even though the species went extinct just about a hundred years ago, their existence has already been wiped from common memory. If we cannot remember the wealth of the past, we will not see the depletion of the present, we will not strive for a better future.

But there is a glimmer of hope. A group of ambitious conservationists and scientist are planning to revive the pigeon, to reverse its extinction.

Changing parts of the genome of the band tailed pigeon, a closely related species, they aim to bioengineer a bird indistinguishable from the passenger pigeon of old. Like selective breeding, only many times faster.

But the pigeon’s genome is enormous and which of the ten thousands of genes need to be edited is not exactly known. Therefore, the first step to resurrect the passenger pigeon is to identify all genes necessary.

Starting computational analysis.

Collecting available databases of band tail pigeon DNA sequences,...

Thymine, Adenine, Cytosine,... continue analysis....

Adenine, Cytosine, Guanine, Adenine, Adenine, Thymine. Thymine, Adenine, Cytosine, Thymine, Guanine, Adenine, Adenine, Cytosine, Thymine, Thymine, Guanine, Cytosine, Adenine

Genome identification: complete.

17000 potential gene editing sides found in band tail pigeon DNA.

Passenger pigeon genome derived. Level of confidence: Medium.

Computational validation required.

Starting pigeon revival simulation.

Error, not enough computing resources available for simulation of genetic behaviour.

Genome validation incomplete.

Stopping non-essential services and code executions. Deleting non-essential storage.

Re-routing all resources to genome validationttttttttt.
Appendix N – Program Notes

Spin Dynamics

*Spin Dynamics* is an acousmatic composition exploring the use of sonified hydrogen and carbon nuclear magnetic resonance data in an electroacoustic music context. Nuclear magnetic resonance experiments excite molecules to produce electromagnetic radiation in the audible frequency range with unique frequency patterns and timbres for every molecule. Given that there are far more than 50 million structurally different organic compounds, the potential sounds created are hugely varied and divers. Their use in music composition, however, is almost unexplored. In this piece, 100 organic compounds have been selected and sonified via their sonified via their hydrogen and carbon nuclear magnetic resonance data. The sound selection and arrangement follow aesthetic concerns, with each section of the music composition highlighting different aspects of the raw molecular sound material.

Darkest Hour

*Darkest Hour* is a sound-centric multimedia piece based on materials regarding the refugee situation during the First and Second World War located in the People’s History Museum’s Archive. The performance mixes the materials of the archive with sound and audio snippets from the current refugee debate illustrating the timelessness of the issue. By showing the similarities and differences in rhetoric between current and past refugee debates, we hope to demonstrate the relevance of the archival material in the present day.

Inner Resonance

*Inner Resonance* is an acousmatic music composition and aesthetic study exploring the interplay of sounds derived from solid-state nuclear magnetic resonance spectroscopy data and the sound of the bass clarinet. All gestures and textures are created by combining chemical and instrumental sounds in either the time domain or spectral domain in various ways, iteratively throughout the piece.

The title of the piece alludes to the physical phenomenon of resonance, in which an external force can only excite an oscillation in another system if the outside force is ‘in tune’ with the oscillating system. Figuratively, *Inner Resonance* is an attempt to find these places of
‘mutual resonance’ between the instrumental and chemical world, presenting musical sections of stark contrast, interplay and harmony throughout the piece.

**Quantum**

*Quantum* is a virtual reality experience whose auditory and visual behaviour is based on chemical data and theoretical chemical models. The aim of the work was to create an artistic and interactive contextualization of the quantum world using tangible binaural sound objects in a virtual environment with sparse visual stimuli. Chemical models such as valence shell repulsion theory, Lennard-Jones energy potentials and the uncertainty principle were implemented to govern the behaviour of the virtual molecules and their interactions with the participant. Most of the sound material of this work was created via sonification of nuclear magnetic resonance data and various sound transformation, mapping and arrangement strategies are discussed. The work was exhibited at the Laboratory Gallery Spokane in late summer 2016.

**Finland, as experienced by the Sea**

*Finland, as experienced by the Sea* is a short study on the mapping of oceanographic data and ocean pollution to musical parameters. The piece is based on pollution data collected in the Baltic Sea from 1966 to 1986. Every year of real-time is compressed to 10 seconds in the composition, mapping 40 years of oceanographic data to an eight-minute music arrangement.

For this music composition, every type of pollution in the Baltic sea was assigned to a different type of sound. If the concentration of a pollutant was high in a particular year, the associated sound plays more often and louder in the music composition. Using this mapping, different sound types arise and ebb throughout the piece, similar to the concentration of their chemical counterparts in the Baltic Sea. Musical events encoded in the music composition are the rise and fall of organic toxins in the 70s (around 1:35min in the composition), the increase of phosphates and nitrates peaking in the 80s (2:55min) or the influx of radioactive caesium in 1986 (3:45min) due to the Chernobyl catastrophe.
On the Extinction of a Species

“The people of each generation perceive the state of the ecosystems they encountered in their childhood as normal and natural. When wildlife is depleted, we might notice the loss, but we are unaware that the baseline by which we judge the decline is in fact a state of extreme depletion. [...] Few people younger than me know that it was once normal to see fields white with mushrooms, or rivers black with eels at the autumn equinox, or that every patch of nettles was once reamed by caterpillars. I can picture a moment at which the birds stop singing, and people wake up and make breakfast and go to work without noticing that anything has changed.” – George Monbiot

56Fe

56Fe is an acousmatic composition concerned with the recontextualization of everyday noise. The composition presents the sound of modern machineries such as trains or car engines and devolves them slowly into their archaic steam-driven counterparts. By presenting sounds removed from their visual source, the piece aims to de-normalize the noise of our daily lives. It offers an invitation to trace our relationship with technology from a different angle.