The sound of chemistry: Translating infrared wavenumbers into musical notes

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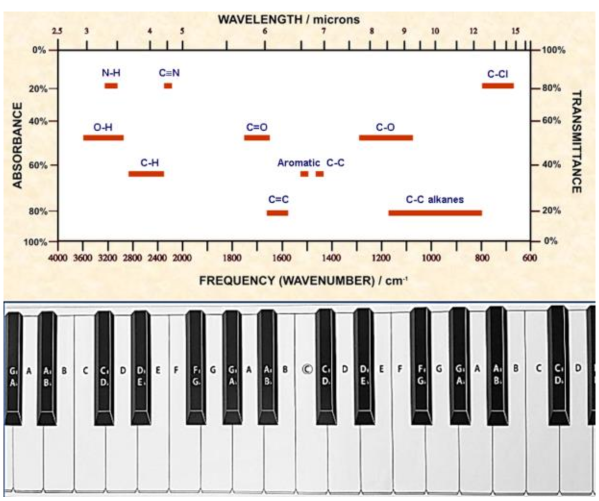
ABSTRACT

The abstract nature of physical chemistry and spectroscopy makes the subject difficult to comprehend for many students. However, bridging arts and science has the potential to provide innovative learning methods and to facilitate the understanding of abstract concepts. Herein, we present a high-school project based on the conversion of selected infrared absorbances of well-known molecules into audible frequencies. This process offered students a unique insight into the way molecules and chemical bonds vibrate, as well as an opportunity to develop their creativity by producing musical pieces related to the molecules they synthesised. We believe that experiencing chemistry from an alternative viewpoint opens up new perspectives not only for student learning, but also for the de-compartmentalisation of scientific and artistic disciplines.

GRAPHICAL ABSTRACT



KEYWORDS
High School / Introductory Chemistry; Public Understanding / Outreach; Multimedia-Based Learning; Physical Chemistry; IR Spectroscopy.

INTRODUCTION

Physical chemistry is traditionally perceived by students as a difficult subject to learn, which leads to low expectations regarding success and negative perceptions of the courses.[1-2] For example, understanding chemical bonding and the use of infrared (IR) spectroscopy to determine the structure of a molecule can be challenging because of the abstract nature of the subject. A study by Sözbilir in 2004 demonstrated that more than half of students perceive the chemical concepts in physical chemistry to be abstract and difficult to grasp.[3] How to increase student interest and how to facilitate learning of such subjects have therefore been of interest for decades.

In this context, the use of audio as a teaching and learning aid is well established, and has a long history.[4-5] As early as in 1974, W. Robert Barnard described some emerging new technologies that could be successfully used for chemistry teaching. Rasul and co-workers recently analysed the effectiveness of audio visual aids in the learning process, and found that it brings a source of motivation for both students and teachers, in addition to several other advantages such as, for example, making the learning process effective, or providing in-depth and detailed knowledge.[6] In particular, the utilisation of music to engage student interest in chemistry is well documented.[7-9] This utilisation spans from incorporating songs in the chemistry classroom,[10] to amplifying biochemistry concepts with content-rich music.[11-12] Amino Acid Jazz, a sing-along exercise in which students synthesise a musical polypeptide from amino acid building blocks, was for example developed by Crowther and Davis in 2013.[11]

From a broader perspective, the use of non-speech audio to convey information (sonification) has been extensively used as a teaching tool, particularly in the context of distance learning since the 1980s.[13] This method is powerful to help students to distinguish differences between sets of data. Some novel ways to present complex data have recently been used via sonification in order to explain very abstract and difficult-to-grasp concepts: For example, Øyvind Brandtsegg offered an insight into the search for quasars (very bright stars) with a musical piece that plays for seven years.[14]

In this broad context, and to go a step further than accompanying chemistry with music to ease the learning of difficult concepts, a closer look at the vocabulary used in physical chemistry in general and in spectroscopy in particular leads to the collection of an interesting set of words: “resonance”, “frequencies”, “harmonics” to name only a few. Those words are also terms used to describe music. The reason for this linguistic proximity is that, although an art, music is by essence of mathematical nature. Chemistry is also describable by mathematics and spectroscopy is a key example of the mathematical nature of chemistry. In theory, it is therefore possible to express chemistry in the language of music (and vice versa), and Kumbar reported in 2007 that “various chemical, nuclear, and biological systems indeed possess the ability to produce some kind of music that is characteristic of their nature”.[15] For example, a first-order reaction will lead to an infrasound type of sound (1×10^{-6} – 1×10^{-2} Hz), whilst an electron transition will make an ultrasound type of sound (1×10^{13} – 1×10^{14} Hz). A limitation of this expression of chemistry in the language of music is that one cannot hear the music produced by the molecules studied since the commonly stated range of human hearing is 20 Hz to 20 kHz.

The link between spectroscopy and music has been studied in the reverse direction. In 2012 Moghimi reported the utility of near-IR spectroscopy for studying the emotional response of subjects to music through analysing the activity of the prefrontal cortex.[16] It is an intriguing symmetry to consider that a music-based emotional response could be generated from spectroscopy.

Therefore, our main questions in the design of this project were: What would happen if we could translate the “sound of chemistry” into the audible range? Could we translate the wavenumbers obtained *via* IR spectroscopy to frequencies we can hear, and if yes, what would be the pedagogical interest of this project?

METHODOLOGY

The synthesis of molecules of interest

The team worked with *ca.* 35 students from Key Stage 5 (Equivalent to US Junior and Senior years). The students were tasked with the synthesis of five molecules (Figure 1): 4-bromo aniline (multistep synthesis from aniline; used in perfumes), *trans*-dibenzalacetone (used in sunscreens), cinnamic acid (cinnamon), aspirin, and phenyl acetate (flavouring ingredient in baked goods and candies). These reactions were of a difficulty deemed reasonable by their chemistry teacher, and offered an interesting range of laboratory techniques from a learning point of view. Along with these five molecules, five other molecules were assigned to the students: carbon dioxide, water, polyethylene, caffeine, and ethanol (Figure 1).

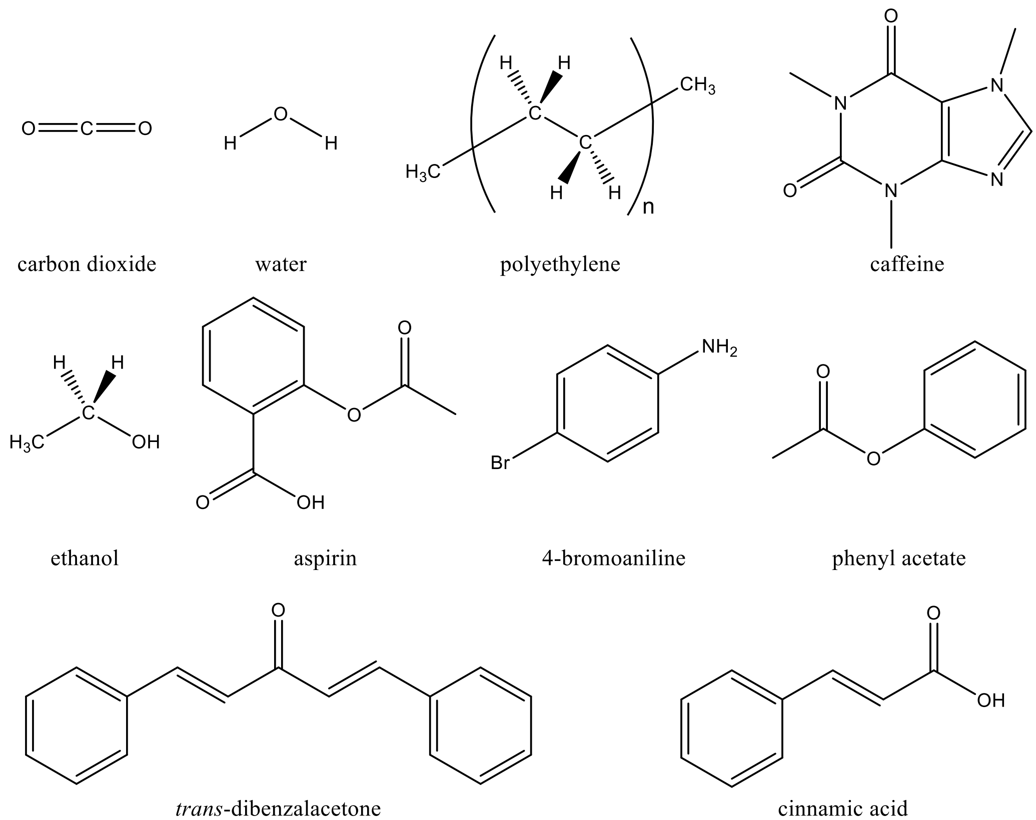


Figure 1. Molecular structures of the molecules studied in this work.

Characterisation of the molecules by IR spectroscopy

The nine molecules (carbon dioxide excluded) were characterised by IR spectroscopy at the university by the high-school students (university staff checked the purity of the compounds by NMR spectroscopy). For practical reasons, the IR spectrum of carbon dioxide was obtained *via* density functional theory (DFT) calculations. The IR spectra of the 10 molecules are shown in Figure 2 (aspirin) and in Figures S1 - S9.

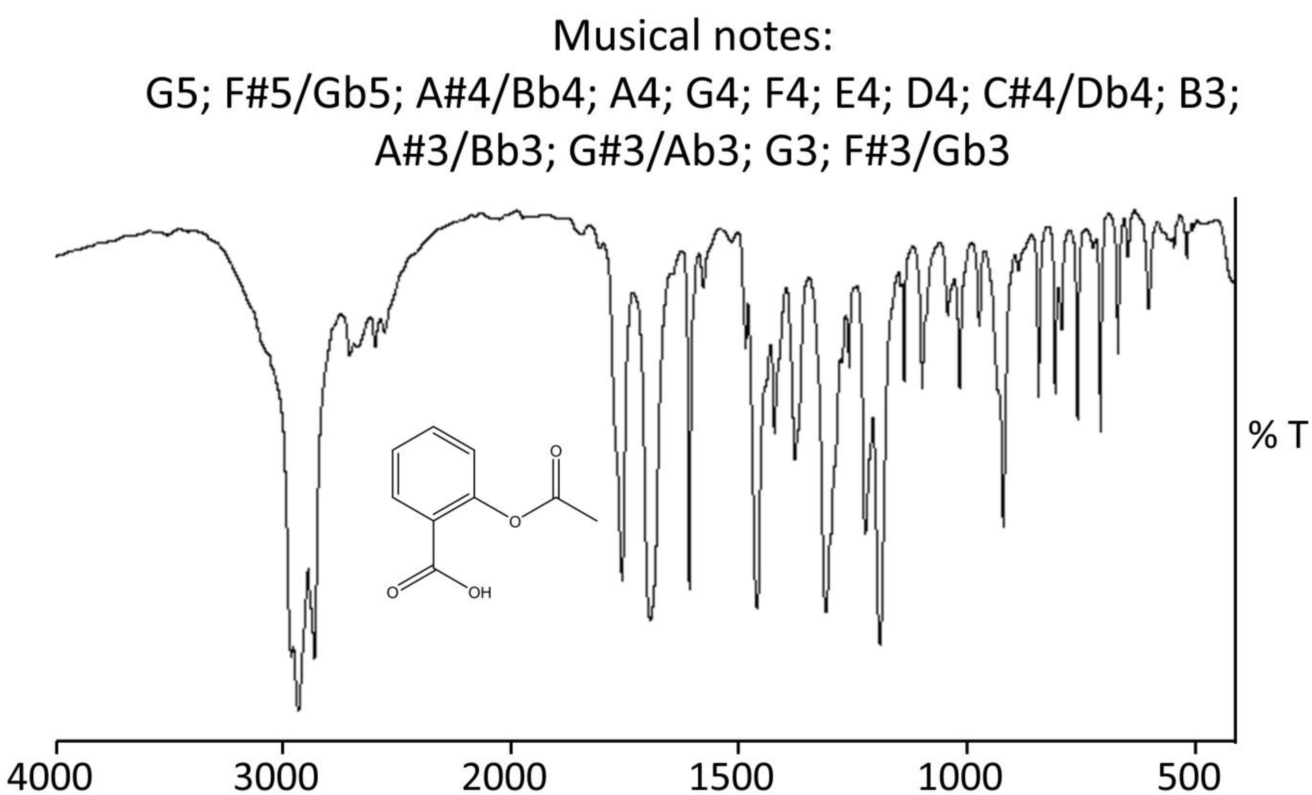


Figure 2. Infrared spectrum of aspirin and unique set of musical notes for the molecule.

Translation of the IR frequencies into the audible range

For each molecule, the key absorption bands were listed in a table in wavenumbers (in cm^{-1}). These were then converted into frequency by multiplying by the speed of light in $cm{\cdot}s^{-1}$, since the relation between wavelength and frequency for electromagnetic radiations is: $\nu = \bar{\nu} * c$ (where ν is the frequency measured in s^{-1} (Hz), $\bar{\nu}$ is the wavenumber in cm^{-1}, and c is the speed of light). A divisor was then applied to convert these key frequencies into the audible range. This coefficient was chosen as it gives a range from C3 to C6 for an IR spectrum run from 500 to 4000 cm^{-1}. The resulting audible frequencies were then compared to the equal-tempered scale (in Hz), in order to associate each IR frequency to a musical note (Table S1). As a result, the characteristic set of IR absorbances for each molecule was translated to a unique set of musical notes (notes are listed in Figure 2 and Table 1 for aspirin; the full spreadsheet can be downloaded as part of the ESI). All the musical notes for the ten molecules are presented in Table 2.

In terms of procedure, peaks were selected by students and inputted into the spreadsheet containing the formula to calculate the notes. Students initially calculated their own mathematical equation to convert wavenumbers into audible frequencies but to have comparison between molecules we used the same factor, provided by the STEM partners. Music students also looked at converting notes using a sliding scale as well as proving the mathematical concept. The students translated the peaks themselves with help from STEM partners.

The peaks selected were across the range of wavenumbers – those that were too small were not selected by the students but it was their choice whether to select the peak or not and they made their own rationalisation for this depending on the compound and the complexity of the spectrum. Absorbances close together mapped to the same note because we were using a standard scale for the notes and not converting directly to a narrow frequency. This meant that any ambiguity was often irrelevant.

Table 1. Example Key Wavenumbers of Aspirin with Translated Frequencies and Musical Notes for the Molecule

Key Wavenumbers of Aspirin, cm^{-1}	Translated Frequencies, Hz	Corresponding Musical Notes for Aspirin
2821.6	65.41	G_5
2649.2	69.30	$F^{\#}_5/G\flat_5$
1749.8	73.42	$A^{\#}_4/B\flat_4$
1678.8	77.78	$A^{\#}_4/B\flat_4$
1604.9	82.41	A_4
1456.0	87.31	G_4
1293.4	92.50	F_4
1182.5	98.00	E_4
1093.9	103.83	D_4
1012.2	110.00	$C^{\#}_4/D\flat_4$
915.0	116.54	B_3
839.3	123.47	$A^{\#}_3/B\flat_3$
753.7	130.81	$G^{\#}_3/A\flat_3$

703.6	138.59	G_3
666.3	146.83	$F^{\#}_3/G\flat_3$

Table 2. Musical Notes Obtained for the 10 Molecules Studied

Molecule	Notes[a]
Carbon dioxide	B_4; $C^{\#}_3/D\flat_3$
Water	F_5; E_4
Polyethylene	$D^{\#}_5/E\flat_5$; D_5; $D^{\#}_4/E\flat_4$; D_4; $D^{\#}_3/E\flat_3$; D_3
Caffeine	$G^{\#}_5/A\flat_5$; G_5; $A^{\#}_4/B\flat_4$; A_4; $G^{\#}_4/A\flat_4$; G_4; G_4; G_4; $F^{\#}_4/G\flat_4$; E_4; $C^{\#}_4/D\flat_4$; C_4; $G^{\#}_3/A\flat_3$; E_3
Ethanol	A_5; $G^{\#}_5/A\flat_5$; G_5; G_5; $F^{\#}_4/G\flat_4$; D_4; $C^{\#}_4/D\flat_4$; $A^{\#}_3/B\flat_3$; F_3
Aspirin[b]	G_5; $F^{\#}_5/G\flat_5$; $A^{\#}_4/B\flat_4$; $A^{\#}_4/B\flat_4$; A_4; G_4; F_4; E_4; D_4; $C^{\#}_4/D\flat_4$; B_3; $A^{\#}_3/B\flat_3$; $G^{\#}_3/A\flat_3$; G_3; $F^{\#}_3/G\flat_3$
4-bromoaniline	F_5; F_5; E_5; $D^{\#}_5/E\flat_5$; E_4; D_4; D_4; C_4; $A^{\#}_3/B\flat_3$; $G^{\#}_3/A\flat_3$; D_3; C_3; $G^{\#}_2/Ab_2$; F_2
Trans-dibenzalacetone	G_5; E_4; $D^{\#}_4/E\flat_4$; $D^{\#}_4/E\flat_4$; $C^{\#}_4/D\flat_4$; B_3; G_3; $D^{\#}_3/E\flat_3$; $C^{\#}_3/D\flat_3$
Cinnamic acid	$D^{\#}_5/E\flat_5$; $D^{\#}_5/E\flat_5$; D_5; D_5; C_5; C_5; E_4; E_4; D_4; C_4; C_4; B_3; G_3; $F^{\#}_3/G\flat_3$
Phenyl acetate	$D^{\#}_5/E\flat_5$; $F^{\#}_4/G\flat_4$; E_4; $D^{\#}_4/E\flat_4$; D_4; B_3; $G^{\#}_3/A\flat_3$; $F^{\#}_3/G\flat_3$

[a]The use of # or ♭ was dependent on the musician's choice of key. [b]See Table 1 for more detail.

Composing musical scores from unique sets of musical notes

The final step of the project was to compose pieces of music for each of the ten molecules. Ten compositions were created (downloadable as part of the ESI, or streaming from reference[17]).

The translation of the IR frequencies into the audible range and the musical compositions were a collaborative effort between the group of chemists and the group of music students. Indeed, although the synthesis of the chemicals and the actual compositions were done separately, the discussion afterwards about the whole process was very much a collaborative process. Chemists discussed the thought process behind the musician's take on the music. They also learnt a bit about the software the musicians used.

Chemists did not have a large role in creating the music but the IR peaks and how IR spectroscopy works was explained by the chemists to the music students. They also discussed what the actual chemicals were used for – for example caffeine's role as a stimulant (more discussion for the more obscure molecules – less so for things like water). Both groups of students also found the caffeine extraction where musicians and chemists went through the whole process together a really useful way of collaborating and sharing ideas (from both sides of the project). Chemists liked the process of having to work 'live' to get the IR spectra of caffeine converted to pass on to the musicians was good as the whole process could be demonstrated quite easily as they worked alongside each other. Chemists inputted in between versions of the music to see how that music should sound to best represent the molecule.

Working exclusively with the musical notes from a given molecule, the students drew their inspiration from various sources. For example, one of the musicians (inspired by both Chopin's Raindrop Prelude and the theme of Inspector Morse) wrote: "H_2O was challenging with only two notes! In the composition, the F5 spells out Water in Morse code and the E4 spells out H_2O in Morse code. There is a motif of a dripping tap constantly dripping in the middle ground and a drone with drums." The sound of caffeine is more upbeat, whilst the ethanol one reflects the depressant effect of the molecule. The sound of aspirin also reflects the effect of the molecule on the human body, with painful discordance in the early stages of the piece before harmony slowly building up to illustrate the healing power of the molecule.

PEDAGOGICAL DISCUSSION

Since Kolb formalised the theory of experiential learning in 1984,[18] the idea that "learning as an outcome is non-learning as ideas are not modified" has been well-accepted. This leads directly to Kolb's cycle which informs of the key point to this style of learning – that learning is continuous and lifelong. The further implication is that: "No two thoughts are ever the same as experience *always* intervenes".[19] Perhaps the most intriguing aspect regarding Kolb's theory was the presence of the dialectical tensions inherent in the cycle – that in order to complete a full cycle one has to reconcile two very different ways of looking at and experiencing the World. Kolb's thesis was that learning occurred when these internal conflicts were resolved, and that it was the teacher's role to facilitate this resolution. Experiential learning is a foundation in chemistry courses from the introductory-level course to upper-level courses through laboratory experiences. Donaghy and Saxton reported in 2012 the benefits of service learning (a type of experiential learning) for the provision of general chemistry courses.[20] Hutchison and co-workers reported that experiential learning help to promote systems thinking in chemistry.[21] The evaluation of the pedagogical impact of this project was therefore of paramount importance for us to determine the validity of this project as a potential experiential learning instrument.

Two different types of high-school students took part in this project: A-level students in Chemistry and A-level students in music. The group of chemists performed the reactions in the laboratory, thereby learning skills which may prove useful should they continue in Chemistry at university level. This project allowed the synthesis of compounds usually not undertaken at high-school level (*e.g.* synthesis of 4-bromoaniline - undergraduate type of chemistry) partly because of the collaboration with University lecturers, but mainly because of the motivation provided to the students by the “next step”. This “next step” (recording the IR spectra, translating the vibrations to obtain musical notes, and composing a piece of music) may be seen as the first application students really do with a chemical. It is obvious for an academic that a compound is synthesised in order to advance towards this particular application (*e.g.* catalyst, drug, etc) but for a high-school student a compound is synthesised because their teacher tells them to. Having this extra motivation of doing something with the compound made the group of chemists really engage with the syntheses in the laboratory. The second benefit for the students was the in-depth understanding of IR spectroscopy gained throughout this project. The concept of absorptions occurring at resonant frequencies became obvious when it had been related to a guitar string vibrating to give a particular musical note. The discussion of why particular bonds absorb IR radiation at a particular energy was also aided by the musical input to the work. Students could clearly understand that a stronger bond, leading to a higher wavenumber absorption in the IR would lead to a higher frequency musical note. Thus, a theoretical concept could be genuinely experienced; a key part of Experiential Learning.

The group of music students also benefitted from this project. Over the months, their approach towards the chemicals studied changed. At the early stages of their involvements, they were looking at the set of musical notes without thinking about the chemicals. However, when they started putting the notes together, they became interested in the properties of the chemicals in order to give a sense to the music, a theme. It was clear at the end of the project that the music students were familiar with the concept of molecular bonding, IR spectroscopy, and their interests in science were renewed. This was particularly evidenced when the team presented their work at the Royal Society Summer Science Exhibition 2019 (RSSSE). The RSSSE is the flagship event of public engagement for The Royal Society and more information about the Exhibition can be found in the Supporting Information. A total of 12,653 visitors came to the exhibition in July 2019. Our stand was one of 22 exhibits only, and included both chemist and music students. Some of the feedback we received from The Royal Society highlights the engagement of the music students with the visitors, thereby evidencing the interest they found in understanding the chemical concepts *via* this project. One visitor wrote: "Very good engagement especially as they are school children. Was even approached a lot and asked if I need to know anything! Even though it required a few rounds of thinking to really decipher the point that notes correspond to chemical peaks, this is complicated stuff and the teenagers managed to explain it well!"

EVIDENCE FOR STUDENT LEARNING

All of the students who did the project had opportunity to complete a project evaluation questionnaire one month after the project finished (in July 2019) and over the summer break from school. This questionnaire was comprised of a mixture of open and closed questions to elicit a good mixture of quantitative and qualitative data, full ethical clearance was gained from the University of Bradford and from the school to approach the students to complete it. Fifteen students completed the questionnaire yielding a 42.8% (43%) response rate; this is acceptable with regard the norm of internal surveys in educational settings achieving a 30-40% response rate.[22] In this project the number of respondents does not need to be considered with regard power as there was no inferential testing of the results.

The students who completed the questionnaire self-reported very positive impacts as a consequence of taking part in the activity: 100% (n = 15) felt that the activity had made a difference to them, and the mean score of how enjoyable it was on a 0-10 scale = 9, with no scores below 8. 100% (n = 15) of respondents said they would recommend the activity to a friend on account of it being variously fun, interesting, educational and challenging. The most frequently cited reasons for considering the project to be valuable included: that the project improved students' knowledge, understanding and skills with regard both chemistry and doing research; that it increased their interest in chemistry and gave them a very special insight into doing chemistry at a higher (i.e. undergraduate) level and as a profession; that the interdisciplinary nature of the project was important, and that they had learnt valuable dissemination skills in terms of being able to speak about the science to audiences.

In terms of impact on pupils' understanding of scientific concepts and skills acquisition, 73% (n = 11) saw themselves as having a better understanding of the science because of the activity. Specifically, 87% (n = 13) reported feeling more confident with regard understanding and using the spectrometer, and 73% (n = 11) reported a positive change in their understanding of infrared energy causing chemical bonds to stretch and bend. Fewer respondents thought that the activity had impacted their understanding of how IR spectroscopy allows us to distinguish between molecules, or that bonds will absorb IR energy at different wavenumbers depending on the composition of that bond, or that IR can be used to monitor the appearance and disappearance of key functional groups – but even so these concepts were better understood by some pupils as a consequence of the activity. Views about chemistry were also reported as positively changed: the data from this open-ended question yielded qualitative themes around appreciating the creative nature of chemistry; that - due to the interdisciplinary nature of the activity - chemistry and the arts were not as poles apart as first thought, and that it was clearer what higher level (i.e. university) chemistry would be like.

93% (n=14) of respondents reported that the project has shown them that people can be *both* scientific and creative, with 80% (n= 12) considering that the music making aspect of the project was important. The reasons given for this were many but included how the music aspect enhanced (*i.e.* made more accessible, made more attractive) the chemistry learning. Again the links between chemistry and music were also valued, as was the chance to work with students in a different department.

In short, it is clear that students valued the project for the ways in which it enhanced their understanding of specific chemistry concepts, exposed them to advanced equipment and techniques, and gave them insight (and in some cases ambition and aspiration) with regard university level chemistry study. The interdisciplinary science-arts hybrid nature of the project was also highly valued with the student appreciating the linkages between the distinct subject areas: it is clear that this was quite revelatory for some pupils, and interesting ideas as to future science-arts hybrid projects were shared.

CONCLUSION

Using music to enhance the engagement of students with difficult concepts in chemistry has been explored for many years, while the relationship between the mathematics of music and chemistry has also been investigated. In a novel approach, we integrated both aspects in one project by translating the vibrations of molecular bonds into the audible range in order to produce a unique set of musical notes for any molecule or material. The project was found enjoyable and helpful for understanding abstract concepts by both chemist students and music students. Furthermore, the impact of bridging arts and science also resonated with the general public, the media (*e.g.* BBC radio 4,[23] The Economist radio[24]) and artists (*e.g.* the Canadian artist and ballet dance teacher Dominique Girard interpreted the sound of 4-bromoaniline[25]). There is scope to extend this project by using UV-visible spectroscopy to add light to the sound obtained by IR spectroscopy for example, or to use this methodology to familiarise groups of people with chemistry. All of us can relate to music and can feel music. This is therefore a perfect medium to create a space for everyone to make the connection between the nature of molecules and the inherent beauty of Nature.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.XXXXXXX. Example of spreadsheet used to translate IR wavenumbers to musical notes and music files for each of the ten molecules discussed in this paper (XLSX)" and "Information about the Royal Society Summer Science Exhibition; Simplified equal-tempered scale in Hz; Infrared spectra for each of the ten molecules discussed in this paper (DOCX)".

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