Class Details

In the following, details of all 16 classes are provided in overview tables. For each class, a summary of the content, the key topics and themes, the learning objectives, the intended course of class progress, and the discussed example cases are listed. This shall help instructors identify easily which of the classes are relevant for their particular course. The headline colour indicates the category of the class: Introduction and summary are grey, classes 2-4 on methodological aspects of good chemistry are orange, classes 5 to 9 on good scientific practice are blue, and classes 10-15 on societal and environmental impact of chemistry are green.

Class No.	Class Title
1	Introduction

Summary of content

At first glance, chemistry and ethics have nothing much to do with each other. One is a modern natural science, empirical, analytic, firmly grounded in ever-refined and improved theories, with high creative potential and applicability for improving everyone's life quality. The other either reminds us of common-sense folk morality or of dry, dusty, intellectual armchair philosophy. Where do these two disciplines – or: attitudes of making sense of our life world – meet? Professional chemists, like all practitioners, ask themselves many normative questions, often without noticing it: What does it mean to do my job well? What is good professional practice? What is the right thing to do in cases of conflicts or dilemmas? Does my work have an impact on society and environment, and is there anything in my responsibility to do about it? Indeed, especially for young chemists, finding answers or solutions for these questions may be much harder than solving chemical challenges like reaction mechanisms, spectrometric analyses, or practical experimental laboratory work.

Before going deeper into these matters, this introduction chapter attempts to explain and clarify some important basic considerations upon which the rationale of this book is built. It will explain the structural division into the three parts methodology, good scientific practice, and social/ environmental impact. It will introduce the role of ethical and normative reflection and make sure that every reader understands that ethical integrity does not require a degree in moral philosophy, but a mindful attitude, clear reason, goal-oriented discourse skills, and the motivation to act professionally as a responsible member of society and, more than that, as an influential and impacting decision-maker in academia, industry, or public service.

Key Themes	Learning Objectives
What is professionalism? When is chemistry (a) *good*? → Right methodology; → Good scientific practice; → Social/environmental impact. Ethics, morality, normativity. Interplay of facts and norms. The ethical prism. Discourse skills. Rationale and structure of this book.	After this class you will… …understand the logic structure of the book, judge the significance of its themes and topics, and be able to select those chapters that matter for your own personal purposes. …be able to explain the difference between ethics and morality and use the implications of these definitions in real-life discourses. …be aware of the touching points between chemistry, society, and ethics. …be prepared for many subsequent discussions using terminology and concepts that are, usually, unfamiliar to chemists and chemistry students.

Course of progress

Step	Task	est. time
1	Reflection: What is a good chemist? (draw and discuss in forum)	15 min.
2	Pre-assessment: What have you heard about already?	3 min.
3	Video lecture, part 1: Dimensions of *Good Chemistry*	22 min.
4	Reflection: What is ethics?	10 min.
5	Video lecture, part 2: Definition of *ethics, normativity, discourse*	12 min.
6	Reading assignment: Mehlich et al., CEJ 2017	20 min.
7	Video lecture, part 3: Course organisation, literature advises	10 min.
8	Reflection: Personal interests and expectations on this course.	5 min.
9	Quiz	5 min.

Class No. 1	Class Title Introduction

<u>Discussed cases</u>

Case 1.1 - Knowledge or Opinion?

At a courtyard, an analytic chemist presents the results of a report that investigates the ground water contamination in a wildlife sanctuary which is most likely originating from a nearby lacquer and paint manufactory. These findings shall serve as an evidence for the company violating environmental regulations. To his surprise, the chemist's evidence-based arguments are countered by the defence as *'one of many opinions*'. The company's lawyers claim that the ultimate proof that the contamination is coming from the manufactory is lacking (*'correlation is not causation*!'), and that science, '*merely based on theory*', would not be able to contribute much to this case that is about the usefulness of legal frameworks, about desirable economic social benefits, and about consumer's life quality.

Case 1.2 - Truth or Dare

In the research group of Prof. X, two Master students A and B, a PhD candidate C, and a postdoc D share a lab. Prof. X assigned postdoc D to supervise student A while the PhD student C is asked to take care of student B. Student A often feels ridiculed and even bullied by D who regards students as immature foolish kids, looking down upon them. Thus, A's trust in D is low. At the same time, A observes that PhD student C encourages B to manipulate experimental data ("It is just for your thesis! Like this it looks more beautiful! Don't worry, X won't notice it!"). Yet, A knows that C would use at least parts of B's experiments for a research paper. A plans to talk to Prof. X about this after a group meeting. In this meeting, however, Prof. X expresses his admiration for his "best students" B and C. Since A's own work, partly due to the poor supervision and support from D, is lagging, she doesn't dare to seek the conversation, worrying about being judged as a troublemaker and risking her grade.

Case 1.3 - Not My Business?

A chemist who is working for a globally operating trade organisation is processing a tricky case: Several tons of thiodiglycol were ordered by a company in Syria, a country recently ridden by civil war. The company claims to operate in the textile industry. Yet, its origins and structures appear hidden and dubious. The trader's chemical background knowledge is good enough to tell that thiodiglycol is, at the same time, a precursor for mustard gas and nerve gas. The seller of the chemical, excited by the excellent business prospect, claims that it is not his or the trader's responsibility to question the communicated application of the chemical (textile manufacturing). Yet, given the low trust in the credibility of the Syrian regime, the trader has severe pricks of conscience to agree to this transaction.

Case 1.4 - The Moral Finger

In a class on research ethics, a student raises concerns about the empiric rigidity of ethical claims. "*Science is truth, but ethics is just opinion, kind of random!*" Thus, he claims, a course like this is useless, because it can't teach knowledge like a chemistry class, but only doctrine and ideology, like the morality finger that warns us not to do wrong. Since he doesn't enjoy the class at all, he stands up and leaves.

Class No.	Class Title
2	Science Theory

Summary of content

Scientific researchers and practitioners, in the context of their profession, take many things for granted. Most scientists, for example, are naturalists and metaphysical realists. In a more hidden way, researchers often follow reductionist approaches in experimental designs and the interpretation of obtained data. Scientific inquiry is, moreover, often said to be a viable source for universal truth claims, based on facts, free from ideology and dogma, and even value-neutral.
Some chemists (basic researchers, academic scientists, university scholars) regard their main job as generating knowledge of the material world, a mission of discovery (*What? When? Where?*) and sometimes explanation (*How? Why?*). Others (chemical engineers, applied researchers, private sector science) add a creative component of exploiting the chemical knowledge we acquired over the century for the creation of something new, something that has not been part of the natural world before.
Knowledge and truth are issues for epistemology, the *knowledge of knowledge*, one of the major disciplines in academic philosophy. It is a central part of philosophy of science and science theory. Admittedly, it is not necessary for a scientist to study and know all this theory. Yet, a bit of it – the quintessential conclusion, perhaps – will surely make the chemical scientist and researcher a better practitioner. Therefore, this chapter attempts to introduce epistemology in a nutshell: What are knowledge, truth and meaning, what is science able to contribute, and when should the chemist be aware of limits and pitfalls of scientific knowledge? The practical relevance for the conduct of chemical science and its application in industry and innovation shall guide the short tour through this complex topic.
It is not a co-incidence or stylistic choice that the key themes below are questions. It is notoriously difficult to settle epistemological debates with definite answers. It may be unsatisfying for chemists, but this chapter's main goal is to raise awareness of questions that challenge beloved convictions and comfort zones. The result is more careful practice in scientific inquiry, and a reasonable balance between epistemic humbleness and confidence, that means knowing the strengths and limits of scientific knowledge.

Key Themes

What is scientific knowledge?
Does science make truth claims?
Do scientists have to be naturalists and realists?
Is science universal, or rather paradigmatic?
What role does meaning play?
What role does education play?

Learning Objectives

In this chapter, you will learn…

…what it means to gain knowledge about the world, and how changes in our understanding of knowledge also change the way we characterise scientific inquiry,
…what presuppositions science is built upon,
…why communication and discourse are crucial for the validity of scientific claims,
…that science is a powerful instrument for the generation of reliable knowledge that is threatened by contemporary developments towards post-factualism and political or religious ideology,
…what the limits of science are, and how a change of theoretical perspective can improve scientific inquiry.

Course of progress

Step	Task	est. time
1	Introduction case: Albertus Magnus vs. Linus Pauling	10 min.
2	Video lecture, part 1: Epistemology in a nutshell	25 min.
3	Reading assignment: Wilhelm Ostwald (Ziche 2012)	30 min.
4	Video lecture, part 2: A Tree of Knowledge	40 min.
5	Discussion case: The Lysenko case (Reading material: Sheehan 2005)	25 min.
6	Quiz	5 min.

Class No. **2**	Class Title Science Theory

Discussed cases

Case 2.1 - Alchemy vs. Chemistry

The alchemists of Europe's late medieval age applied Aristotle's theories and principles in their investigations of Nature and its components. They intended to transmute cheap metals or even stones into gold and to find the formula for immortality. With simplest means, polymaths like Albertus Magnus collected samples of minerals and organic materials, experimented with them, identified patterns and resemblances, catalogued, filed and indexed. But no matter how hard they tried, there is no reported case of successful gold fabrication or immortalisation. From today's perspective, it seems quite ridiculous to assume that it was possible. Yet, we may ask on what grounds the alchemists had the conviction that is was possible.

Case 2.2 - The Politics of Molecules

Wilhelm Ostwald was a German chemist in the late 19th and early 20th century. Besides his chemical achievements, for example the famous Ostwald dilution law and his colorimetry research, he was a declared monist who believed that there are universal principles underlying everything from nature and its laws to human behaviour to society with its spheres. For example, he promoted his energistic conception of molecular forces as directly applicable to how politics should work: a constant harmonizing of attraction and repelling forces balancing each other out in the naturally most stable form. People in a society, if governed properly, find their most suitable position like the atoms in a stable molecule. Is this a plausible view?

Case 2.3 - Chemical Dogma

The Russian biochemist Trofim Lysenko was in charge of advancing post-WWII Russia's agriculture program. He had the enthusiastic support of Joseph Stalin which he maintained by applying Stalin's voluntarist approach to the governance of social processes to chemical experimentation and its interpretation. Unfortunate for him, his proposed and realised measures to increase the output of Russia's agriculture failed utterly and almost caused a famine.

Case 2.4 - Who knows?

Xhrk is a bronze age human and member of a clan in which he is assigned the role of a weapon smith. His father showed him where to find good raw material for the alloy fabrication and how to cast blades, but he found by himself that adding charcoal to the fire in which the ore is molten increases the stability of the weapon. John is a chemistry student who just received a good grade in the inorganic chemistry midterm exam. After studying the recommended textbook thoroughly, he could explain the chemical reactions involved in alloy manufacturing flawlessly. Who has knowledge about alloys? Xhrk, John, both, or none of them?

Case 2.5 - Shift work

Thomas Kuhn is famous for his work on science theory, especially his view that science revolves around *paradigms*. A predominant paradigm is guiding the work and thought of scientists in a way that results are interpreted in favour of it, until a sufficiently large number of counter-evidences has been collected to shift the paradigm to a better alternative in an inevitable *scientific revolution*, as Kuhn calls it. That means, scientific progress is not a smooth increase or advancement of knowledge, but a step-like change of understanding that requires force and, possibly, power. An example is the Bohr-Sommerfeld atomic model that helped explain many observed effects until too many deviations and inconsistencies were detected so that it was given up by the scientific community and replaced by a better model. Can you find more examples that would support Kuhn's view? Are there examples that would suggest that Kuhn is wrong?

Class No.	Class Title
3	The Scientific Method

Summary of content

In chapter 2 we have seen how scientific inquiry can be characterised, distinguished from other ways of knowledge construction, and that scientifically acquired knowledge has a high chance of being viable, reliable, and of withstanding critical scrutiny. It examines aspects of our natural world and enables evidence-based factual statements and judgments. But how can we make sure that a statement is *scientific* in a sense that it fulfils certain requirements of scientific knowledge generation? What is the method with which scientists come to insights that deserve the label *scientific*? This chapter and the next aim at describing all the features that make scientific research such a powerful way of gaining viable insights.
After identifying the basic steps of a scientific investigation and their characteristics in terms of typical activities of scientists and researchers, a systematic step-by-step guide through the elements of a chemical research project is presented in the form of Lee's scientific knowledge acquisition web. Key issues are the formulation of hypotheses, the analysis and interpretation of experimental results and data, appropriate strategies in cases of errors and encountered difficulties, record keeping, and reporting and publishing considerations. While this chapter discusses conceptual and methodological issues, it defines the arena of good scientific conduct and helps enlightening the standard of what counts as *good*. Thus, it lays a foundation for chapters 5 to 8.

Key Themes

One method or *many methods*?
Elements of scientific methodology:

- Designing research inquiries.
- Making hypotheses.
- Choosing experimental setups.
- Interpreting and analysing data.
- Systematic and conceptual errors.
- Record keeping.
- Reporting and communicating results.

Learning Objectives

After reading this chapter, you will be…

…aware of the steps of scientific research, and the importance of each part of it,
…able to identify where you are with your own research in the scientific knowledge acquisition web, and what this stage requires from you,
…equipped with insights on the difference between scientific researchers and other personnel involved in R&D (like lab technicians, editors and publishers, or engineers),
…able to handle and apply scientific conceptual terminology like theory, model, hypothesis, observation, reproducibility, etc.

Course of progress

Step	Task	est. time
1	Introductory case: Is *Umbrellaology* a science?	15 min.
2	Scientific Inquiry Literacy Test	5 min.
3	Pre-assessment: What are elements of a scientific method?	10 min.
4	Video lecture, part 1: Elements of a *scientific method*	7 min.
5	Reflection: How do you proceed with your own research project?	10 min.
6	Video lecture, part 2: Scientific Knowledge Acquisition Web	35 min.
7	Continue reflection: Forum presentation/discussion	15 min.
8	Quiz	5 min.

Class No. **3**	Class Title The Scientific Method

Discussed cases

Case 3.1 - Money for Nothing?

Gary started his first faculty position as an assistant professor recently. He just received a letter in which the Ministry of Science and Technology announces that his research grant application is rejected. He is extremely frustrated, because he thought he had a very creative research idea: A novel catalytic pathway to synthesise planar cyclobutane derivatives. After an institute meeting, an older colleague approaches him and offers help with drafting another grant proposal. His experience, as he claims, is that such grant proposals always need a clear statement on application potentials. "*You won't get money for nothing! But if it is not curing cancer, tackle climate change, or support sustainable innovation, the ministry guys think it is good for nothing*!". Now, Gary is wondering if research ideas are really better when they have practical purposes as their goal.

Case 3.2 - Dead End

Julia, a PhD student in a research group that does supramolecular chemistry, is trying to functionalise cyclodextrin vesicles with short protein chains since more than a year. Even though her PI mentioned that this project is more like an exploration of an unknown and uncertain territory, she wishes to have at least some successful experiments. But nothing seems to work as planned. She tried hundreds of variations of synthesis conditions. Now she is at a point where she feels like throwing it all away and ask her PI for another topic for her thesis, not only because of her grade but also because it seems it is a waste of resources, material and money to continue with this hopeless project. Yet, there is always this slight bad feeling that the failure is due to her own incompetence…

Case 3.3 - It doesn't work!

Ian is trying to synthesise an amine-based dendrimer that is equipped with a fluorescent marker. A comparable compound can't be found in the literature. Short amines can be coupled with the fluorophore, but it seems not to work with common reaction conditions when the amine is a large dendritic molecule. The other option, building the dendrimer arms after coupling the core amine with the fluorophore, doesn't yield complete but only irregular dendrimer products. After 4 months of trying several approaches, his best outcome is a yield of 15% of the final product. This is good enough for his purposes. Yet, he starts wondering whether he should include all the failed attempts in his research paper. Otherwise, someone else who is not satisfied with this yield will try all the other methods again that Ian knows are less promising. Isn't it necessary to publish negative results in order to avoid useless repetition of experiments that don't work and to make scientific research more efficient?

Class No.	Class Title
4	Scientific Reasoning

Summary of content

Besides the technical and experimental skills in daily lab work and a profound knowledge of one's professional field, chemical researchers need competence in analysing and interpreting their acquired experimental data in view of the claims they made in their research hypotheses. Both - making proper hypotheses and interpreting data in a scientific manner - are topics in this chapter. First, it will introduce the most important concepts of logic that play a role in scientific thinking and reasoning: Deduction, induction, and abduction. More important than the correct application of logic concepts is the awareness of pitfalls, biases and fallacies. Then, we will learn how logic informs the heart of the scientific method, the predictive power of proper hypotheses and the explanatory power of data analysis and interpretation. Furthermore, a subsection is dedicated to heuristic and methodological analysis. Last but not least, it is worthwhile to have a closer look at statistical analysis and the differences between frequentist and Bayesian approaches.

The goal of such a chapter in a book on good chemistry is, of course, a higher awareness of factors that determine the consistency and plausibility of scientific claims. In intra-community discourse among scientific experts, but also in extra-community communication with non-expert stakeholders or the public, argumentation and the logically correct positioning of evidence-based facts decide over the success of the proposed claims. This is not only essential to come to viable – that means, pragmatically true – knowledge, but also to maintain credibility and trust in the force of scientific methodology. Furthermore, it gives a foretaste of chapters 5 and 6 in which we will elaborate in greater detail what is good scientific practice and what is scientific misconduct. Many types of misconduct and fraud are, in one way or another, the intendedly fallacious or undermined application of scientific reasoning.

Key Themes	**Learning Objectives**
Deduction, Induction, Abduction; Logic errors, biases, fallacies; Prediction and Explanation; Causation; Heuristic and methodological analysis; Frequentist and Bayesian statistics	This class is intended to equip you with… …basic logic skills for scientific thinking and reasoning, …the competence to identify and avoid biases and fallacies, …strategies for heuristic and conceptual analyses of hypotheses and research questions, …awareness of the importance of statistical analysis, …the ability to think and argue clearly with scientific concepts.

Course of progress

Step	Task	est. time
1	Warm-up question: George Berkeley's *Esse est percipi* in chemistry?	5 min.
2	Introductory case: The Calabrese case (Shrader-Frechette 2014)	20 min.
3	Video lecture, part 1: Logic and scientific reasoning	36 min.
4	Further information: Bayesian vs. Frequentist Statistics (youtube video)	25 min.
5	Watch the video, 36:29-45:21	10 min.
6	Discussion: The Baltimore case (Reading: Lang 2015)	20 min.
7	Watch the video, 45:22-end	10 min.
8	Quiz	5 min.

Class No.
4

Class Title
Scientific Reasoning

<u>Discussed cases</u>

Case 4.1 – Certainly uncertain

An analytic chemist is conducting toxicological studies on functionalized nanoparticles. These are designed to serve as imaging agents for the detection of joint inflammation (arthritis). None of the tests, so far, indicate any detrimental physiological effects. Moreover, a critical component, a short protein receptor on the NP's surface coating, can't be detected in free form, which means that the composition of the NPs is stable. When communicating the results to the medical partner who will conduct clinical tests, her formulations are questioned. The doctors wish to have certainty that the NPs' chemical composition and stability is safe for patients. Is the toxicologist able to claim this degree of safety with sufficient certainty?

Case 4.2 – Spectral proof

At a group seminar, a PhD candidate announces the successful synthesis of a new compound. The PI, though, is not satisfied since the student's only analytic result is an H-NMR spectrum that shows at least two uninterpretable peaks ("dirt") and in which the assignment of one hydrogen atom in the molecule deviates from the expected value. The student argues that the mass spectrometry of this compound is difficult due to decomposition reactions in the spectrometer, and that a CHN analysis is ambiguous. Yet, as most of the group members agree, having only one indication of the successful synthesis of the product, it is very likely to interpret it too benevolently and with a bias.

Case 4.3 – Just call it 'Proof of Principle'!

Ryan used a chemical deposition technique to fabricate a field effect transistor. The precise and flawless formation of the different layers of semiconducting, isolating, and conducting materials is notoriously difficult. Finally, on one of his specimen, he is able to perform electronic measurements that show the field effect. When he tries to repeat the measurement, he is not able to locate a suitable spot for the attachment of the circuit wires. His PI is satisfied, anyway. It was successful once, that means it works! In the paper, it will be declared a *proof of principle*!

Class No.	Class Title
5	Scientific Misconduct

Summary of content

In order to reach the goals of scientific inquiry, a set of behavioural attitudes and *virtues* must be complied with. Acting in contrast to or violation of one or more of these scientific virtues is *scientific misconduct*. Many cases of downright fraud have been reported throughout the history of science, some of which are individual criminal intent, while others are the result of character dispositions amplified by systemic pressure. Some cases are not only a matter of research ethics, but also illegal. Fabrication of data, falsification of data, and plagiarism are forms of cheating, betraying and stealing, and, thus, can be sanctioned in institutional and legal terms. Other cases like the omission of data, the post-processing of images, copying experimental instructions from other sources, etc., are debatable, but not clearly illegal or unethical.

This chapter has two purposes: It wants to show that scientific misconduct is a real problem in the chemical community, and it wants to give guidance for the decision whether an intended action in a research context is appropriate or not. The former received a lot of media attention, lately. More importantly, empirical studies on the behaviour of scientists have been conducted, so that data on misconduct is available. The more difficult question is the reason for fraud and misconduct. It is worth enlightening at least some of the motivations so that an awareness of them can protect from falling victim to them. The latter purpose is a matter of discourse. We will see how the science virtues can help making the right decisions for oneself, but also protecting others from slipping into the dark side of betrayal and fraud by seeking goal-oriented mature conversation. Empirical studies have shown that training in research ethics doesn't make researchers commit less fraud. But whistleblowing does! Paying attention to one's surrounding and finding proper strategies to address misconduct is, arguably, the most efficient way to ensure the community's scientific integrity.

Key Themes

Research ethics as virtue ethics → Virtues of "good science". Scientific integrity.
Misconduct as intended fraud, biased motivation, or deliberate sloppiness.
FFP cases (fabrication, falsification, plagiarism), grey zone cases.
Reasons for and prevention of misconduct.
Whistleblowing.

Learning Objectives:

If you take this chapter serious, you will…

- …be able to make arguments in favour of or against certain practices – your own or observed on others – on the basis of the virtues of good scientific practice, thus giving them justificatory power and yourself more confidence and, subsequently, positive influence,
- …be aware of the possible forms of misconduct that are frequently reported and that are constantly around the corner as options for chemical practitioners,
- …not fall into the trap of believing that fraud and misconduct can bring you any benefit,
- …know how to address forms of misconduct and make convincing arguments that explain in which way they are wrong,
- …bring forward these arguments as a whistleblower without risking your own integrity.

Course of progress

Step	Task	est. time
1	Warm-up question: Everyone cheats?	10 min.
2	Introductory case: Bengü Sezen (Schulz, C&EN 2011)	10 min.
3	Video lecture, part 1: Virtues of science	19 min.
4	Reading material: Fraud in science (Martinson et al. 2005)	10 min.
5	Video lecture, part 2: Data falsification, fabrication, plagiarism	7 min.
6	Further information: Robert Millikan (youtube video)	25 min.
7	Video lecture, part 3: Millikan, grey zones, reasons for fraud	19 min.
8	Quiz	5 min.

Class No. 5	Class Title Scientific Misconduct

Discussed cases

Case 5.1 - Swear the Baconian Oath!
Jenny and Peter discuss a newspaper report about recent fraud cases in scientific research. They come to the agreement that scientists, indeed, have quite a huge impact on society and, thus, a high responsibility for doing their job well. Peter thinks that the current institutional guidelines for good scientific practice are enough. When people have the 'criminal energy' to violate them, anyway, it is rather a structural or systemic error of how we organise science institutions and their individuals. Jenny, on the contrary, thinks that researchers' social impact makes them almost like medical doctors. Thus, she insists, after their education and before they start their jobs, they should prove their ethical integrity by swearing an oath in analogy to the Hippocratic Oath of doctors. With Francis Bacon as the forefather of the modern approach to science, we could formulate a Baconian Oath for scientists!

Case 5.2 – Bengü Sezen
[Real case] Reports from Columbia University and the Department of Health & Human Services (HHS) show a massive and sustained effort by Bengü Sezen over the course of more than a decade to dope experiments, manipulate and falsify NMR and elemental analysis research data, and create fictitious people and organisations to vouch for the reproducibility of her results. She was found guilty of 21 counts of research misconduct by the federal Office of Research Integrity (ORI) in late 2010. Amongst other things, she logged into NMR spectrometry equipment under the name of colleagues, merged NMR data and used correction fluid to create fake spectra showing her desired reaction products. How is this possible, both in terms of Sezen's personality/psyche and in terms of peer assessment by colleagues, co-workers, supervisors or manuscript reviewers?

Case 5.3 – The Baltimore Case
[Real case] In the late 1980s, MIT Prof. David Baltimore's PhD student Thereza Imanishi-Kari and postdoctoral fellow Margot O'Toole had a disagreement on the validity of data that served as the basis of one of Imanishi-Kari's papers. O'Toole believed to have found discrepancies on 17 pages of one of Imanishi-Kari's lab notebooks. In a first instance, Imanishi-Kari was found guilty of 'serious scientific misconduct', leading to the retraction of the paper. Yet, a federal prosecutor decides not to prosecute her for fraud because of the complexity of the case making it impossible for the jury to judge. Not much later, the ORI concludes that she did fabricate data. The HHS bars her from receiving federal funds for 10 years. However, it revokes this decision after a HHS panel finds that the ORI didn't prove misconduct. Why is this case so complicated? What role does record-keeping play, here?

Case 5.4 – Millikan, the betrayer?
[Real case] In 1978, historian Gerald Holton reported that Millikan omitted data without apparent reason when publishing his famous oil drop experiment in which he determined the charge of an electron. This could be a case of fraud. Indeed, out of the 107 valid drops listed in his lab notebooks, he reports only 58 in the publication. 27 of those not published have been dismissed after calculating *e*. For at least 5 of these Millikan's notes don't explain his decision to omit them. Critics claim that the only apparent explanation for the omission is that they didn't fit Millikan's expectation. How can it be decided whether this is a case of misconduct?

Class No.	Class Title
6	**Scientific Publishing**

Summary of content

We have learned that communicating scientific findings is a crucial step of scientific methodology. Scientific claims gain their universal validity only through passing critical review by fellow experts. Besides doing science, *writing science* is one of the main activities of researchers and scientists. Thus, it is not surprising that many cases of scientific misconduct are committed in the context of publishing. Authorship decisions, citation practices and plagiarism, but also peer review and the benefits and dangers of impact factors are frequently discussed among chemists. This chapter focuses on the intra-community aspects of scientific publishing, whereas chapter 15 addresses issues of public communication of chemistry. The issues in that field are very different.

We will see how the scientific virtues introduced in chapter 5 can inform decision-making and discourse on publishing issues. Fairness, disciplined self-control, and communalism play the most important role in this context. Yet, self-interests can cause biases that impact the choice of authors for a paper, the choice of references given in an essay, the review process of competitive papers, or publishing practices that increase a researcher's visibility in the form of impact factors. A special topic, here, is the publication of research that has obvious dual-use potential and is, thus, controversially discussed.

Key Themes	**Learning Objectives**
Doing science vs. writing science; Authorship; Citation practices; Peer review; Impact factors; Predatory Publishing; Publishing controversial research	This chapter supports you in… …getting aware of publishing-related ethical issues, …learning possible solutions for arising conflicts like authorship discussions or peer review problems, …applying the virtue approach to publishing-related professional conduct, …becoming a responsible member of the scientific community by engaging in improving the fairness and ethical integrity of practices like peer reviewing and impact factors.

Course of progress

Step	Task	est. time
1	Pre-assessment: Publish or perish?	5 min.
2	Introductory case: Predatory publishing (reading material: web articles)	15 min.
3	Video lecture, part 1: Publishing research, overview	23 min.
4	Reading assignment: Citation and Carbon allotropes (Hoffmann et al. 2016)	30 min.
5	Video lecture, part 2: Citation practices	12 min.
6	Discussion case: Peer review	20 min.
7	Video lecture, part 3: Peer review, impact factors, controversial research	23 min.
8	Workshop: Submission for publication	15 min.
9	Quiz	5 min.

Class No. 6	Class Title Scientific Publishing

Discussed cases

Case 6.1 – The unknown collaborator

Belinda just published her first research paper. She wrote the first draft, including the introduction, the experimental section, and the discussion of the results. Her PI 'polished' the paper and submitted it. After being accepted, she receives the 'proofs', and to her surprise there is an author X on the list of whom she had never heard before. Immediately she consults her PI to ask about X who, according to the information on the paper, works at another university. Her PI says that X is a friend and collaborator who contributed to this paper by inspiring him to do this research and also "*reviewed the introduction and suggested some changes*". Yet, Belinda finds, the introduction as printed in the proofs is almost 99% identical with her first draft. She assumes that her PI adds X as a personal favour. Yet, since X may increase the visibility of the paper with his name, she doesn't object it. However, when she presents a poster at a conference a few weeks later, another researcher approaches her and inquires about her collaboration with X: "*It is really interesting that you worked with X! What is your experience with him? Have you visited his labs? Pretty amazing equipment, right?*". She feels embarrassed and has tough times finding the right replies.

Case 6.2 - Temptation

While writing a research paper on the kinetics and mechanism of a novel organic catalysis reaction – a project that required hard work and included a good postdoc and the best PhD candidate – Prof. Smith receives an article to review for the *Angewandte Chemie* journal. To Smith's horror, the paper, written by a senior colleague at another university, reports the same reaction. Apparently, she has been faster! Smith knows that he could simply raise objections to the paper and delay its publication for months, giving time to submit his own article to another journal. On the other side, working on a very similar project, he knows that the colleague did very excellent work, actually.

Case 6.3 – Careful with that pox, Eugene!

[Real case] Ryan Noyce, Seth Lederman and David Evans published the complete chemical synthesis and fabrication of the horsepox virus in January 2018. Immediately, concerns have been raised that this information can be used to construct variola, the virus that causes the eradicated disease smallpox. In a response to the objections, communicated in October 2018, they argue that (1) available knowledge is not sufficient, but the construction needs skills that require advanced scientific training and insider knowledge that is not widely available, (2) that the benefits of the availability of this synthetic virus (developing vaccines) outweigh the risks, and that (3) there are no regulation issues since the research team has thoughtfully obtained all necessary legal reviews of relevant legislation. Is this convincing enough to dispel the worries concerning bioterrorism and biosafety?

Class No.	Class Title
7	Chemistry as a Network Activity, Part 1: Academic Chemistry

Summary of content

Chemistry is - on several levels - teamwork, and as such embedded into a wide network of actors and stakeholders. This chapter will focus on issues that arise in the context of collaborations and co-operations across these levels. We will see what kind of conflicts can arise when chemists work with fellow chemists (including PI-student interaction and mentorship), with other natural scientists, or with completely different scientists (social sciences, humanities).

Every network of people is, almost necessarily, also a network of interests. Sometimes, these interests overlap, and people pull in the same directions. Yet, at other times, interests clash, and collaborative work becomes inefficient, exhausting, or unfair. Throughout the career as a chemist, whatever that career looks like, every chemist faces various situations that bear risks of conflicts and dilemmas. For most of us, the first time is the research work in a professor's group as graduate or PhD students. Besides conflicts arising from personality dispositions and competition, an important aspect is the power imbalance between mentor and student. Both mentor and student need skills in professional communication and conflict solving to reach their goals to the satisfaction of both. At all stages of the chemical career, multi-, trans- and inter-disciplinary collaborations, nowadays, are rather the rule than the exception. These span a wide variety of experts, non-experts, interest groups and stakeholders, posing different challenges on the conduct of the chemical practitioner. This chapter attempts to apply the scientific virtues of chapter 5 to this realm of professional integrity.

Key Themes:

- Chemistry as teamwork.
- Harms:
  - power,
  - conflicts of interest.
- Mentoring.
- Multi-, trans-, inter-disciplinary collaborations.

Learning Objectives:

After this class you will be…

…a better mentor/superior, or a student/inferior with the ability to solve conflicts with convincing discourse skills and good arguments,

…a better collaborator with high scientific integrity, communicative skills and positive influence,

…an open-minded interdisciplinary bridge builder that can see beyond the narrow margin of your own professional expertise and competence.

Course of progress

Step	Task	est. time
1	Warm-up reflection: To cooperate, or not to cooperate?	10 min.
2	Introductory case: Compete or collaborate?	15 min.
3	Video lecture, part 1: Chemistry as network activity	22 min.
4	Discussion case: Proper mentorship	15 min.
5	Video lecture, part 2: Mentorship	15 min.
6	Exploration: How interdisciplinary is the chemistry department of the University of Bayreuth?	20 min.
7	Video lecture, part 3: Multi-, trans-, inter-disciplinarity	10 min.
8	Creative task: Types of collaborations	15 min.
9	Quiz	10 min.

Class No.	Class Title
7	Chemistry as a Network Activity, Part 1: Academic Chemistry

Discussed cases

Case 7.1 – No love!

Prof. Miller has a very strict rule for students joining his research group: He doesn't allow love-relationships between two members of the group. If two form a couple, one must leave the group. For some students, this is reason enough not to join Prof. Miller's group. Some think that it intrudes the students' privacy and that it is not a professor's business how close his students are with each other. Yet, after making bad experiences with couples in his group, leading to trouble and low work efficiency whenever the couple had private problems, he claims that he has good reasons to establish this rule. Is this appropriate leadership and mentorship?

Case 7.2 - Truth or Dare (Case 1.2 revisited)

In the research group of Prof. X, two Master students A and B, a PhD candidate C, and a postdoc D share a lab. Prof. X assigned postdoc D to supervise student A while the PhD student C is asked to take care of student B. Student A often feels ridiculed and even bullied by D who regards students as immature foolish kids, looking down upon them. Thus, A's trust in D is low. At the same time, A observes that PhD student C encourages B to manipulate experimental data ("It is just for your thesis! Like this it looks more beautiful! Don't worry, X won't notice it!"). Yet, A knows that C would use at least parts of B's experiments for a research paper. A plans to talk to Prof. X about this after a group meeting. In this meeting, however, Prof. X expresses his admiration for his "best students" B and C. Since A's own work, partly due to the poor supervision and support from D, is lagging, she doesn't dare to seek the conversation, worrying about being judged as a troublemaker and risking her grade.

Case 7.3 – REACHing a goal together!

[Real case] With the rise of nanoscaled substances and their industrial application since the early 2000s, the maintenance and management of a chemical registry became extremely complex and practically difficult. The European Chemical Agency, tasked by the European Commission to conceptualise and implement a new chemical registration and supervision regulation, faced this challenge. What competences are needed for this endeavour? Why can't it be accomplished by chemists alone? Yet, in which way is chemical expertise necessary for a viable outcome?

Class No.	Class Title
8	Chemistry as a Network Activity, Part 2: Private-sector chemistry, Science policy

Summary of content

In the previous class we talked about some aspects of chemistry as a network activity. We learned about group-internal conflict potential (for example, in mentoring) and different forms of collaborations with other scientists or academic disciplines (for example, interdisciplinary co-operations). In this class, we turn to two instances in the network that are outside the academic community: Governance (and its role for chemistry), and industry. Typical ethical issues arising in these contexts are conflicts of interests, academic freedom in the light of contemporary science funding practices, and intellectual property right protection. Necessarily, we will extend the scope of research ethics to issues of business ethics and profession ethics.

Key Themes

- Chemical R&D and Innovation in the private sector, difference to academic chemistry.
- Source of conflicts: Intellectual property issues.
- Impact of science policy and funding on academic freedom.

Learning Objectives

After watching/listening to/reading this class, you should be able to…

…identify potential conflicts of interests that underlie your motivations for and decision-making in your research activities and collaborations;

…help solving conflicts in your academia-industry collaborations with proper goal-oriented argumentation based on scientific integrity;

…maintain a reasonable balance between interest- and purpose-driven science (topics that are promising for acquiring funding) and academic curiosity-driven basic science;

…identify your main interest (for example doing something useful for society, understanding the material world, advancing knowledge, performing experiments) and choose your future job wisely.

Course of progress

Step	Task	est. time
1	Warm-up reflection: Whatever makes you happy?	5 min.
2	Case: Misuse of public funding?	15 min.
3	Video lecture, part 1: Chemistry and politics, public funding	17 min.
4	Discussion: Academic freedom at threat?	15 min.
5	Case: Conflict of interest	15 min.
6	Video lecture, part 2: Academia and industry collaboration	17 min.
7	Assessment: COIs at your university?	5 min.
8	Case: Intellectual property violation	15 min.
9	Video lecture, part 3: Intellectual property	10 min.
10	Activity: Create a wiki on copyrights	15 min.
11	Quiz	10 min.

Class No.	Class Title
8	Chemistry as a Network Activity, Part 2: Private-sector chemistry, Science policy

Discussed cases

Case 8.1 – Money matters!

Graduate student Alan is working with Dr. Lee on a DFG-funded (German Research Foundation, public) research project on mass spectral identification of biomolecules. Yet, after starting the work, Dr. Lee is asking Alan to study a series of organometallic cluster compounds which are important in industrial catalysis but have no direct biological significance. Upon Alan's inquiry, Dr. Lee explains that, if the project works, she would be able to obtain contract funding from major oil companies which is important in times of tight government funds. Alan wonders whether it is acceptable to be paid from the DFG grant but work on something very different. Dr. Lee says that she would be able to make up a good biochemical reason for Alan's work, and that the project manager would never know the difference. "*Everybody does it like this!*".

Case 8.2 – Not my ligand!

[Real case] Two students in the same group were funded by different companies with individual confidentiality agreements. Student A was trying to find new homogeneous catalysts for a particular reaction; student B was trying to find new uses for a particular ligand. Student A asked the supervisor if it would be OK to use student B's ligand (provided by the company funding B) in the reaction being studied. The supervisor agreed to allow the use of student B's ligand by student A and it gave better results than any other. Without naming the other company, both companies were informed. They were both extremely upset and threatened legal action. In the end, they agreed that the IPR should be taken out by the company funding student B. The company who funded student A never funded more research in the group (after about 15 years of continuous funding) whilst the other company continued to fund the group. If student A had used a commercial sample of the ligand rather than the sample that had been supplied by the company funding student B, there would have been no problem.

Class No.	Class Title
9	Animal Experiments

Summary of content

Admittedly, not all chemists face the situation of conducting animal experiments at any time in their career. Yet, those who do often struggle with ethical concerns about the justification of animal use in research and regulatory testing, see themselves confronted with public outrage, and face a load of paperwork that legislators request in order to limit animal sacrifice to a reasonable minimum. The bioethical considerations that inform the discourse on animal experiments easily exceed the competence of scientific researchers, toxicologists and analytic chemists in academia, industry and public service. At the same time, in practical terms – public debate and regulatory requirements – animal experiment practitioners can't escape the obligation to understand at least roughly what is at stake.

The goal of this chapter is to refine bioethical theory into an applicable overview of arguments that researchers can use as orientation for their daily discourses and experiments. The virtue ethics approach of the previous chapters is not sufficient for that. Instead, a brief introduction to bioethical reasoning strategies will give the reader a clearer sense for the conflict potential that the pro and the contra side face. Here, the image of ethics as a prism that was drawn in chapter 1 is very powerful: We are not looking for *the right solution* as the result of an *ethical lens*, but rather attempt to refract the complexity of views into clear and plausible positions and their underlying justifications. It is also in this respect that *every* chemist, not only those who conduct animal experiments, may have a gain from paying careful attention to this chapter. In a propaedeutic sense, getting to know the approaches employed in an ethical *hot topic* like animal research supports ethical reasoning and argumentation competence and prepares for other seemingly intractable conflicts in the discourse on science and research.

Key Themes

Types of animals and purposes of animal experiments on vertebrates; means and ends of animal experiments; bioethics (benefits of outcomes (utilitarian); rights and duties (deontology); anthropocentrism and biocentrism); pro and contra arguments; regulation, 3R guideline

Learning Objectives

Chemists might be affected by the ethical debate on animal experiments in two ways: They find themselves attacked or criticised by opponents of animal testing (sometimes unjustified or unreasonably), or they are asked to follow legal and ethical guidelines for animal experimentation. Thus, in this chapter, two competences are acquired:

- Responding to objections and verbal attacks with proper and plausible arguments, so that credibility is maintained, and argumentation is reasonable and convincing;
- Understanding the ethical background of regulations and fulfilling formal requirements (the necessary paperwork before and after animal experiments) professionally and satisfyingly.

Course of progress

Step	Task	est. time
1	Pre-assessment I: Experience with animal experiments and its debate?	5 min.
2	Pre-assessment II: Opinion on animal experimentation?	5 min.
3	Opening discussion: PETA on animal treatment	15 min.
4	Reading assignment: Animal testing (Olsson, Sandoe 2012)	20 min.
5	Video lecture, part 1: Arguments	42 min.
6	Activity: Moderate a talk show discussion	20 min.
7	Discussion case: Considering alternatives	20 min.
8	Video lecture, part 2: Regulations and requirements	10 min.
9	Further reading: The ECHA website on animal testing	10 min.
10	Quiz	5 min.

Class No.	Class Title
9	Animal Experiments

Discussed cases

Case 9.1 - Bad Publicity
A medium-sized company produces paints and lacquers as consumer products. Innovative new products need approval in terms of dermatological innocuousness and environmental safety. As regulations require, the former aspect was tested in cooperation with an analytic institute that conducted animal studies as part of an EHS assessment (environment, health, and safety). The company got into the focus of a local animal rights activist group that hired a reporter to publish a not so benevolent article on the animal cruelty case in this company. The next day, a crowd of upset protesters gathers in front of the manufactory facility and confronts the head of the unit, a chemist by training, with accusations of animal torture. The heated atmosphere threatens to escalate.

Case 9.2 - Standing Ground
A popular TV talk show hosts a discussion panel on animal testing. The debaters are:
- A toxicologist conducting animal experiments for basic research;
- A CEO of a cosmetics company (known for testing their products on animals);
- An animal rights activist protesting against any form of animal experiments.

The scientist faces aggressive opposition from the activist, but gets support from the CEO. At the same time, he feels sympathy with the activist's concerns and despises excessive animal use for regulatory testing of luxury consumer products which, for him, is different from the reasonable occasional conduct of animal experiments for the purpose of scientific insight on species ecology and biomedicine.

Case 9.3 - Evaluating Alternatives
A graduate student is asked by her PI to order 15 mice in order to perform a series of experiments investigating the possible mutagenic effects of a newly synthesized class of compounds. Although quite common in her discipline, having never considered non-human animal experimentation necessary to her research, the student suggests that perhaps these experiments wouldn't be necessary. The PI emphatically disagreed and, in response, explained that while non-human animals may potentially experience suffering throughout the study, this was an essential and inevitable part of scientific research. It would be more important, the PI reasoned, to safeguard the health of humans who would later come in contact with these compounds in the future than those animals that were bred specifically for this type of research. Given a few days for the design of an experiment that would minimise the suffering of the mice, the student finds alternatives in the literature. Machine learning of toxicological big data from the REACH database has been used to predict and verify the hazards of tens of thousands of known molecules. Also, there are protocols in place that use cell cultures rather than mice. The student remains conflicted. As suggested by her PI, non-human animal experimentation seems to be the fastest and most well-established methodology to investigate these new compounds, while the alternatives carried their own sets of risks and consequences: unknown transferability, highly-specialized skills, longer experiments and greater cost.

Class No.	Class Title
10	Chemistry and Values

Summary of content

In this part 3 of the book, we attempt to understand the impacts that chemical activity has on society and environment. With the same application-oriented approach of the other two parts, we will focus on the role that chemical professionals play in the network of actors and decision-makers. Yet, first, it is necessary to show in which way chemistry is not per definition neutral or value-free. It is not difficult to see how chemical industry, private sector R&D and innovation, but also regulation and governance of chemical progress, have social and environmental implications that can be assessed and *evaluated* (thus, necessarily, implying *values*). For chemistry as academic science and research it is not that obvious, though. Therefore, we will outline the ties between chemical science, technology development, innovation, and how progress is embedded in the social and cultural lifeworld of the people that it effects. Moreover, the chapter will introduce the contemporarily predominant social constructivist view of S&T progress by a short historical comparison with earlier paradigms. This will help us understand why reflecting on normative dimensions of scientific and innovation activity is not trivial or waste of time, but an important element of research on how to make S&T progress sustainable and beneficial.

Key Themes

- Chemistry as social sphere;
- Chemistry as science and/or technology driver;
- Neutrality theses;
- Dual use;
- Technological determinism vs. social constructivism.

Learning Objectives

This chapter shall convince you that…

…scientific activity is not neutral or value free but embedded in social practices and normative frameworks,

…science is a main driver and facilitator of technological development, and as such subject of the same ethical considerations,

…an ethical evaluation can't start at the application level where it has a visible impact on society and environment, but must start at the early development level (scientific research) in order to identify and push trajectories of development that are desirable and beneficial.

Course of progress

Step	Task	est. time
1	Pre-assessment: Neutrality of science?	5 min.
2	Introductory case: The Case of Agent Orange (Galston, 1972)	20 min.
3	Video lecture, part 1: Neutrality of science?	31 min.
4	Reading material: Social and ethical dimensions of sciences (Develaki 2008)	20 min.
5	Video lecture, part 2: Social construction of science	20 min.
6	Discussion: Should scientists serve the common good? (Reading material: Ioannidis Interview, 2015)	20 min.
7	Quiz	5 min.

Class No. **10**	Class Title Chemistry and Values

Discussed cases

Case 10.1 – Manhattan Project
[Real case] The standard textbook example for social responsibility of scientists is the Manhattan project, including Einstein's letter to US president Roosevelt, and the role of basic researchers like Oppenheimer. Since the discovery of nuclear fission by Otto Hahn and Liese Meitner in Germany in 1938, its scientific investigation and subsequent application was firmly connected to the historical political situation. Almost immediately after it became clear what incredible forces it could unleash, scientists (!) expressed concerns about the chance that Nazi-Germany could develop a weapon that exploits the devastating effects of nuclear fission. Under the leadership of the US government, thousands of scientists and staff worked on winning the race of being the first to have a nuclear bomb. Three weeks after the first successful test, two nuclear bombs were dropped on Hiroshima (August 6th 1945) and Nagasaki (August 9th 1945), killing 180,000 people instantly and probably up to 300,000 in the following years through radioactive contamination. Otto Hahn considered suicide after hearing the News from Hiroshima. The scientific leader of the Manhattan project, Robert Oppenheimer, quitted the project right after the bombs have been dropped on Japan and fought against the further development of nuclear bombs, especially the hydrogen bomb. He was then accused of disloyalty by the US government.

Case 10.2 – Agent Orange
[Real case] Arthur Galston discovered a chemical compound, 2,3,5-triiodobenzoic acid (TIBA), that inhibits the growth of leaves and, instead, increases the number of floral buds on soybean plants. In higher concentrations, though, it leads to defoliation (abscission of leaves) and the death of the plant. He learned later that the US army, interested in this chemical's defoliation effects, produced derivates of this compound and used the most powerful ones (known as *Agents Orange*, *White* and *Blue*) in the Vietnam war, having disastrous effects on the ecosystem, food chains, and the aboriginal culture and lifestyle. Galston remained extremely concerned about the implications of his work, not shying away from confrontation with the US government. He became a public voice of science that reminded fellow scientists of the inherent dual use potential of every scientific discovery. "*The only recourse for a scientist concerned about the social consequences of his work is to remain involved with it to the end!*"

Case 10.3 – Boom!
[Real case] Prof. K. from M. is doing research on nitrogen-rich compounds that have promising potential as explosives. In papers and presentations, he explains their application in mining, construction industry (for example, tunnels) and space rockets. A closer look at this profile reveals that most of his work is funded by the army. It is obvious that most of his compounds are of interest in warfare products (missiles, bombs, landmines, etc.). Confronted with the dual use potential of his work, he states: "*See, I am just the scientist. I only deliver knowledge about how things work. I am not the one to tell others what to do with it. Of course, I envision that my explosives will make somebody's life easier, for example the miner or the engineer. I can't judge whether a war is justified or not, and I also can't see how my chemical compounds would have any implication for that question*."

Class No. 11	Class Title Sustainability

Summary of content

In the previous chapter, we outlined the role of values and societal factors in and for scientific and other chemical activity (research, innovation, industry, business). We have seen that the complexity of the debated issues can overwhelm professionals and practitioners with chemical expertise to a point that any ethical or social consideration is rejected and delegated to other actors and stakeholders. The overall goal of this chapter is to systematise and, thus, *tame* the discourse on values implicit in S&T development. The most prominent, most widespread and best accepted approach is *sustainability*.

In recent years, sustainability became a key concept in environmental and social politics, both on local and global levels. However, it is often not clear what people exactly mean when they use this term and what it particularly implies. Let's try to bring a bit of light into it. Please keep in mind that we do this because we want to understand it as the reason for reflecting on ethical aspects of S&T progress. The principles of sustainability will give us a framework for the evaluation of risks and benefits of S&T.

This chapter sets the scene for the following chapters. It is necessary to understand that evaluations of risks, responsibilities, desirable or undesired developments of science and technology proceed in professional realms (governance, commissions, academic and economic decision-making) in discourses among stakeholders on the basis of plausible principles of justice and fairness. Generally, the question is "*How do we want to live, and how can we make sure that future generations also have the freedom to ask this question and decide upon it?*". This is the idea of sustainability.

Key Themes

Concept and definition of sustainability;
Sustainability as a normative framework for S&T discourse;
Sustainable chemistry;
Sustainability and ethics:

- values in the *Sustainable Chemistry* discourse;
- sustainability as value co-creation;
- needs and necessities.

Learning Objectives

Upon completion of this chapter…

…you as an actor in S&T development - here: a chemical professional - understand what sustainability implies and what it means in practical terms for your job;

…you can evaluate various stakeholders' interests, identify overlaps and conflict potentials, and mediate between different values applying principles of justice and fairness in your decision-making;

…you have the skill to analyse the consequences of your decisions in terms of sustainability, so that related processes (in R&D, in industry, in economy) become, indeed, sustainable.

Course of progress

Step	Task	est. time
1	Warm-up reflection: My own research project and sustainability	10 min.
2	Reading assignment: Sustainable and Green Chemistry (Albini, Protti 2016)	15 min.
3	Video lecture, part 1: Definition of sustainability	33 min.
4	Further information: Chemical leasing (youtube video)	10 min.
5	Video lecture, part 2: Chemical leasing	4 min.
6	Reading material: REACH and sustainability (read only chapter 2 of the provided report, the rest is optional)	20 min.
7	Video lecture, part 3: Sustainability and REACH	10 min.
8	Discussion/reflection: Chemistry and Sustainability	15 min.
9	Quiz	5 min.

Class No. 11	Class Title Sustainability

Discussed cases

Case 11.1 - Competing Interests
A metal-working firm produces metal parts that come out of the production process with a greasy film. Before shipping them to their clients, they must be cleaned using a solvent. This solvent is purchased from a chemical supplier. The amount of used solvent is rather large due to inefficient cleaning procedures, spillages and workers' incompetence in carrying out the cleaning procedure. The supplier, yet, seems reluctant to support the metal-working firm in solvent handling since an increase in efficiency would go along with selling less solvent. The result is more chemical usage than necessary, higher costs, higher risk in transportation, storage and disposal of the solvent, higher environmental burden. Is there any way to reduce the solvent usage without violating any actors' interest (including the supplier's)?

Case 11.2 - Chemical Complexity
The result of synthetic chemistry as a productive creative process is a large and ever-growing amount of new compounds and substances with potential applications in industrial and academic R&D. Safety regulations demand that all chemicals that workers, users and third parties possibly get in touch with must be properly characterised and handled. Yet, once a chemical registry is maintained, it is already outdated and incomplete. How can the gains and objectives of a chemical registry – safety, completeness, correctness, feasibility – be weighed with the exorbitant requirements on its maintenance? How can a reasonable load of scientific and administrative work power best be invested in creating a chemical data base that supports industry, R&D, business AND the wider public?

Case 11.3 - Whose value?
Geologists have located a large amount of a rare earth element rich ore. Unfortunately, its mining would immensely affect a national park that is one of the last protected natural habitats of an endangered animal species. The mined resources are industrially extremely important, used worldwide in IT consumer goods, generally believed to increase life quality and global equality. How can the economic and social values be compared to or weighed with the environmental values (biodiversity, health of the ecosystem, etc.)? What role can and do chemists play in the discourse on such problems and their practical solutions?

Class No.	Class Title
12	Responsibility

Summary of content

Chemical activity (science, research, engineering, innovation) - through its entanglement with technological development - affects and impacts normative and other value-related discourses concerning social and environmental dimensions of S&T progress. It is now time to introduce the concept of responsibility in order to clarify the position of chemists in this discourse.

Many responsibility attributions, especially from the public, apparently, are not justified and mere accusations. Others are justified but chemists might not be aware of them. The difference is often one of a conceptual dimension: Who can be held responsible by whom, for what exactly, and in view of what rules, competences and knowledge? Apparently, responsibility attributions are only legitimate when the agent that is held responsible has the cognitive capability to understand and act in accordance with certain expectations and obligations. Moreover, different types of responsibility need to be differentiated in order to make justified claims: legal, social, political, organisational, and moral responsibilities.

The considerations in this chapter, basically, have two goals. First, it shall help chemical practitioners defining their roles in progress and public discourse. This implies acceptance of some responsibility ascriptions and refutation of others. In any case, plausible arguments are required to claim or reject responsibilities. This chapter will provide such a line of argumentation. Second, it shall convince chemists that their most general responsibility – contributing with their expertise and competence to the collective endeavour of sustainable S&T progress - arises from an obligation to serve the common good.

Key Themes

Four dimensions of responsibility:

- who is held responsible,
- by whom,
- for what,
- in view of what rules or knowledge?);

responsibility vs. accountability;
types of responsibility (legal, social, organisational, moral);
Responsibility ascription to chemists.

Learning Objectives

After studying this chapter, you are able to…

…oversee, and apply, the four dimensions of responsibility attribution,

…respond to unjustified responsibility attributions and accusations convincingly and with proper arguments,

…see more clearly where exactly the responsibilities of chemists as professional actors in academia, industry or governance lie and how they manifest themselves in particular calls for action and participation in public discourse on social and environmental impact of chemistry.

Course of progress

Step	Task	est. time
1	Warm-up reflection: Responsible for… responsible to…	10 min.
2	Introductory case: Agent Orange (revisited)	20 min.
3	Video lecture, part 1: Four dimensions of responsibility	23 min.
4	Reading assignment: Responsibilities of Scientists (Develaki 2008)	25 min.
5	Video lecture, part 2: Chemists' responsibilities	25 min.
6	Discussion cases: Chemical weapons, POPs	20 min.
7	Activity: Reflect on your own responsibility as a chemist, discuss with peers.	15 min.
8	Quiz	5 min.

Class No.	Class Title
12	Responsibility

Discussed cases

Case 12.1 – Complicity in war crime?

[Real case] Dutch chemist and businessman Frans van Anraat sold thousands of tons of chemicals to the Hussein regime in Iraq in the 1980s, among them thiodiglycol, precursor for mustard gas and nerve gas. Chemical weapons that have been produced with his chemicals were used during attacks on Kurds in Northern Iraq in the late 1980s, killing thousands. Van Anraat was arrested and sentenced to 17 years in prison for complicity in war crimes. He himself pleaded innocent, claiming that a businessman is not responsible for what clients do with the deliveries, and that he believed his chemicals were for the Iraqi textile industry.

Case 12.2 – I don't like POPs!

[Real case] A chemist working at the United Nations for the Stockholm Convention on Persistent Organic Pollutants (POPs) gives a talk about his work as an invited speaker at a university symposium. When coming to the responsibility of chemical sciences and R&D, a chemistry professor in the audience stands up, apparently very upset, and complains about the speaker accusing chemists of being the root of all kinds of problems in the world. "*You want to blame us and make us feel guilty! Fine! Then let's stop all chemical research and go back to stone age*!", he declares full of bitter sarcasm. He leaves the room without listening to the speaker's reply.

Case 12.3 – Different view

Matthew, Peter and Conny studied chemistry together 15 years ago and meet again at an alumni meeting of their university. Remembering their joyful study years, they also come to talking about their current situations. Matthew is working in the R&D section of a big chemical company. Peter got a job in an analytic lab of the national environmental protection agency. Conny is an assistant professor at a renowned university. Matthew claims: "*Sometimes I wish I had chosen an academic career! I miss the academic freedom! In industry, in recent years, we have so many restrictions, and expectations on 'responsible research and innovation' and such things! I feel a heavy burden of responsibility!*". Peter objects: "*But it is good like that! I mean, all these regulations are in place to guide chemical progress in the right direction! RRI is a useful tool to help chemists act in responsible ways!*". Conny adds: "*And don't think that academic chemistry is free from responsibilities! All the public scrutiny and the trend towards applied science with its dual use risks don't stop at faculty doors!*".

Class No.	Class Title
13	Risk, Uncertainty, Precaution

Summary of content

Almost all aspects of the discourse on societal and environmental impacts of scientific and technological development can be framed in terms of risk and uncertainty. It is an unavoidable component of progress and innovation that some effects are unpredictable and unknown. Therefore, this topic deserves its own chapter in the context of chemical progress in science, R&D and innovation. Here, we will shed light onto the conceptual and practical definitions of risk and uncertainty, approaches to risk assessment and risk management, the role of chemists in different risk discourse contexts, and contemporary institutional implementation of handling uncertainties in the form of the precautionary principle.

Risk is one of those terms that different people associate with very different things. Chemists – that is, people with an educational background in a natural science, often working in environments in which technical problem-solving by using expertise, knowledge, skills and competences – often understand risk as something empirically comprehensible (for example, the likelihood of a malfunctioning or contamination) or a result of ignorance that can be tackled by doing more research (that means, a cognitive challenge). We will learn that parts of the risk discourse revolve around normative and evaluative aspects. In accordance with the claims in the previous chapters, decision-makers and actors in chemistry contexts benefit from an awareness of these discourses as important contributors to an interdisciplinary endeavour: mitigating risks on a solid evidence-based factual foundation (delivered by science and empirical research) under consideration of a well-informed plausible normative framework.

Key Themes

Definitions of risk & uncertainty;
Risk assessment;
Risk management;
Risk discourse types:

- Simple risk → instrumental
- Complex risk → epistemic
- Uncertain risk → reflective
- Ambiguous risk → participative

Precautionary principles

Learning Objectives:

With the content of this chapter in mind, you will have…

…a sharpened awareness of various levels of risk types and the demands on their respective discourses,

…an idea of the role of chemical scientists and researchers in such discourses,

…the motivation to participate actively in multi-stakeholder discourses in ways that your professional position provides, so that the goal of reducing risks and increasing benefits can be reached.

Course of progress

Step	Task	est. time
1	Warm-up reflection: What does *risk* mean?	5 min.
2	Introductory reading: Chemical risk assessment (web article)	15 min.
3	Video lecture, part 1: Risk definition, risk assessment	22 min.
4	Assignment: My own risk assessment 1 ("classical")	15 min.
5	Discussion case: The Nano-Sunscreen case (Jacobs et al. 2010)	25 min.
6	Video lecture, part 2: Risk discourse types	17 min.
7	Reading assignment: Precautionary Principles in Chemistry (web article)	15 min.
8	Video lecture, part 3: Precautionary principles	10 min.
9	Discussion: My own risk assessment 2 ("The larger picture")	15 min.
10	Quiz	5 min.

Class No. **13**	Class Title Risk, Uncertainty, Precaution

Discussed cases

Case 13.1 – Big issues with small particles

Sunscreens with titanium dioxide nanoparticles are commercially available. Toxicologists could not identify any adverse health effects of the NPs. Based on these studies, consumer products have been approved by regulators. Yet, the success of such innovative sunscreens is below the expectation. Cosmetics companies classify the market potential as risky. Consumerists, too, employ the parlance of risk trade-offs in the discourse on risk and benefits of nano-sunscreens. Was there a misunderstanding?

Case 13.2 - Chemometrics

A good analytic chemist knows that every toxicological study goes along with false positives (for example, a substance showing a certain toxicity in a test while, actually, it is not toxic) and false negatives (a substance showing no effects while, actually, it is toxic). According to textbook knowledge, a threshold should be set where the rates of both types of error are equal, because such a scientific approach should be neutral. Yet, the good analytic chemist wonders if this is plausible. In a real-world context, wouldn't it be safer to overestimate the toxicity of a compound rather than to risk toxic substances slipping through the test? That means, shouldn't the threshold be set in a way that false positives are taken more serious (with bigger impact) than false negatives?

Case 13.3 – Better safe than sorry!

Dr. Philipps works in the R&D department of a chemical company, synthesizing and testing organophosphates and carbonates for application as pesticides. Several of his products are on the market. Yet, he is puzzled about a letter from the management that says that the current procedure of sending compounds for new marketable products to the EPA for approval is now changed because of the enactment of a REACH regulation. From now on, instead of the regulators demonstrating that a product is not safe before removing it from the market, companies have to prove their products are safe before they are introduced into commerce. Dr. Philipps sighs. This requires a big load of extra work and maybe external contractors for the toxicity studies. Probably, this is what *responsible research and innovation* is about: Better safe than sorry!

Class No.	Class Title
14	Science Governance and Technology Assessment

Summary of content

After introducing concepts like sustainability, responsibility, risk, and the connection between scientific activity and ethical values, we still miss a crucial link: Why would this matter to chemists, and what is in their power to do about impact of chemical R&D on society and environment? This chapter will introduce channels and established procedures for chemical professionals in science, research and innovation to contribute with their competence and expertise in the context of S&T governance and policy, in public stakeholder discourse, or in any form of S&T assessment.

In chapter 10, we discussed the Manhattan project as an example for scientists taking social responsibility. Einstein wrote a letter to President Roosevelt to warn him of a threat. Today, scientists don't need to write letters to political leaders. Instead, a variety of communication and exchange platforms have been created. In the European Union and its member states, offices of technology assessment are associated with parliaments or governments in order to inform S&T governance and policy with state-of-the-art scientific knowledge and a competent estimation of the expectable trends of the nearer future. Decision-making in the context of societally important topics like health care, energy supply, mobility, infrastructure, food supply, etc., requires the input from experts who, ideally, are skilled in interdisciplinary discourse and communication with non-experts. After an overview of the role of scientific expertise in policy-making and the implemented approaches for a fruitful contribution, a guide for successful policy-relevant knowledge reporting is presented. The considerations of chapter 1 – the role of ethics as a discourse methodology for the clarification of facts and norms through an ethical prism – become most effective in this chapter.

Key Themes

- The role of scientific expertise in S&T policy and governance;
- Technology Assessment;
- EU research programs' accompanying work packages (ELSI, RRI, 3O);
- Knowledge reporting.

Learning Objectives

This chapter shall help you to…

…set the insights from the previous chapters (sustainability, responsibility, risk discourses) into perspective and understand their meaningfulness and relevance for chemical professions,

…know the possibilities of chemists to engage in S&T-related discourses on desirable and undesirable implications and effects of chemical progress and its role in innovation,

…avoid common fallacies and misunderstandings concerning the role of scientists in such discourses and bring in your competences in the most credible and fruitful way.

Course of progress

Step	Task	est. time
1	Warm-up reflection: The role of science for regulation and decision-making.	10 min.
2	Introductory reading: Nanoscientists in ELSI (Shumpert et al. 2014)	20 min.
3	Video lecture, part 1: Scientific policy-advise	35 min.
4	Activity: Advise your parliament	15 min.
5	Further reading: RRI in a nutshell (web article)	10 min.
6	Video lecture, part 2: Chemists' contribution	15 min.
7	Discussion case: Chemical expertise in tackling plastic pollution of oceans	15 min.
8	Reflection: ELSI assessment of your own research	15 min.
9	Quiz	10 min.

Class No. **14**	Class Title Science Governance and Technology Assessment

Discussed cases

Case 14.1 – We need you!

Prof. Stone is part of a larger multi-national research consortium that develops novel materials for infrastructure construction. The complex grant application with its references to several of the sustainable development goals has been approved by the European Commission, so that the 15 partners from academia and industry receive funding for five years. He can finance three PhD students and a postdoc for research on physicochemical surface coating methods that shall increase the durability of concrete-steel structures in combination with plant cover for green architecture. Unexpectedly, he receives an invitation for a meeting of the *work package on ethical, legal and social implications* of the project from the leader of that WP, a social scientist. What does he have to do with that?! Since his schedule is extremely full, Prof. Stone rejects the invitation and decides that he lets those sociologists do their thing while he does his.

Case 14.2 - Speculation

At the end of the first decade of this millennium (2007-09), a large number of publications and research projects addressed ethical and social issues in the field of nanosciences and nanotechnologies. Many essays were written by authors who themselves are not nanoscientists, and scientific-technical introduction chapters in multi-author books were only loosely connected to the other chapters. This led to the accusation that *nanoethics leaps ahead* and discusses science fiction rather than the real and more urgent developments in state-of-the-art nanoscience. At the same time, national and international technology assessment offices were asked by parliaments and governments to support efficient policy-making with scientific input on ethical, legal and social implications of nanotechnology. How can this dilemma be solved?

Case 14.3 - Don't let me be misunderstood

Prof. Ramirez, leading expert on industrial scale polymerisation reactions for manufacturing of plastics, is asked to speak at a UN panel about the chemical possibilities to fabricate environmentally friendly plastics (for example, biodegradable or recyclable), alongside other experts who address topics like trapping plastic microparticles in water cycles, policies for limiting consumption, or alternative materials from plants like cellulose. Prof. Ramirez is planning his speech which is limited to 10 minutes plus 10 minutes Q&A. How can he explain all the science that is necessary to understand the complexity of polymerisation reactions in large throughput reactors? His students learn that in 8 hours of lecture time. What else would he have to report so that the panel will be convinced of the high economic value of these reactions?

Class No.	Class Title
15	Science Communication

Summary of content

Former chapters pointed out the importance of communication and discourse as an element of the scientific method itself (chapters 2 and 3), communication with peers and members of your scientific community (publications, conference talks) (chapter 7), with collaboration partners and practitioners from outside your own field (class 8), and with regulators, non-expert decision-makers and other stakeholders (class 14). This chapter elaborates further on communication of chemical issues in informal environments or with the general public, either through channels of mass media or face-to-face in public panels or public education (museums, science campaigns, etc.).

The communication between experts and non-experts is always an asymmetric one: Specific knowledge may be misunderstood or not understood at all, and once it is refined for easier comprehension it may be misinterpreted or applied in inappropriate contexts. The dialectic (that means, *in both directions*) requirements on successful science communication in chemistry start with chemical experts' awareness of these obstacles. Chemists who want to reach out of their chemical community, for example giving an interview to a science journalist for a Newspaper, providing scientific advice to a science museum, writing a chemistry book for children, or participating in a public roundtable discussion on climate science, need to practice this form of communication like they train everything else.

In this chapter, we will discuss why competences and skills in public communication of chemical matters are important and necessary, how this competence can be acquired, and how a chemist should listen and respond to non-expert communication partners in the general public. Again we will meet the important differentiation of fact-premises and norm-premises as introduced in chapter 1. Here, it will help us understand the conflict potentials that arise in public communication of an expert field like chemical science, research and innovation in academia, industry, and public service.

Key Themes	**Learning Objectives:**
Science and mass media; Chemists and science journalism; Practicing public communication; Public participation in S&T discourse.	In this chapter, you will learn… …that communication with scientific laymen needs to be trained and practiced in order to avoid pitfalls and common mistakes, …how to respond to public concerns and questions properly, to distinguish scientific knowledge-directed questions from those concerning worldviews and values, and to increase your credibility as an important public figure with competence and influence, …that scientists have an authority to deliver evidence-based factual knowledge that would be filled by others when not actively occupied by scientists.

Course of progress

Step	Task	est. time
1	Warm-up reflection: Layman - who cares?	10 min.
2	Introductory cases: Baking soda as cancer treatment, water memory, chemtrails	15 min.
3	Reading assignment: Why public communication?	20 min.
4	Video lecture, part 1: Public communication of chemistry	24 min.
5	Example case: Explain organic Chemistry (TED talk)	20 min.
6	Video lecture, part 2: Practicing public engagement	12 min.
7	Further information: EU project "Irresistible"	10 min.
8	Discussion case: Advantages from misrepresentation?	20 min.
9	Video lecture, part 3: Scientists in public discourse	16 min.
10	Activity: Write for non-chemists	20 min.
11	Quiz	5 min.

Class No.
15

Class Title
Science Communication

Discussed cases

Case 15.2 - Crosstalk

[Real case] The following is an excerpt of a conversation at a Q&A section of a public information event about nanoparticles for the early diagnosis of arthritis at the Charité hospital in Berlin.

Patient 1: "You say that your particles can visualise the joint inflammation 15 years before the rheumatic symptoms appears?"

Researcher: "Yes, that is correct. The particles have protein receptors that can find special molecules in the joint that indicate an inflammation. That means, they accumulate, and…"

Patient 1: "OK, I got that! But why would I want to know that 15 years in advance when there is no treatment method in place, anyway?"

Researcher: "Aehm… I… I am sure treatment methods are under development, too! But as a first step, it is necessary to identify the inflammation, and with our method…"

Patient 1: "But do I have a right of not-knowing? I mean, what if my employer or my health insurance find out? Can I make sure that I am not in trouble with that diagnose, especially when I show no symptoms?"

Researcher: "I don't know… I am not an expert on patient rights. But our method is safe, there is no indication that the nanoparticles have any adverse effects, so you don't need to worry about the test."

Patient 2: "Well, but in your presentation 5 minutes ago, you said that you don't know for sure where the particles end up! You said, 'probably' they are transported to the kidney and then egested. It means, you don't know, right?"

Researcher: "Right, we can't find the particles after the diagnostic tests, but we also can't observe any negative effects in any of the toxicity tests and clinical trials, which means that…"

Patient 2: "To me, that doesn't sound convincing. I don't think I would have that kind of test when it is not safe!"

Case 15.3 - Not My Business?

A new faculty member has recently begun her research into the development of catalytic anti-cancer metallodrugs. Her focus has been on the role of stereochemistry in the complexes she and her students synthesise to enantio-selectively reduce metabolic intermediates generated in certain classes of cancer cells. Her research is lab-based and she currently does not have any contact with cancer patients nor have her proposed complexes been used in any clinical trials. She would characterize her research program as fundamental science with a focus on the biochemistry of cancers.

Early in her first year as a faculty member, she is invited to a dinner hosted by a local group looking to privately invest 50k € in innovative research from young scientists. The group is comprised of local entrepreneurs with limited scientific training. The group proposes that she should prepare a short 10 to 15-minute presentation for the committee. This video will be recorded and later posted on the organization’s website to highlight the innovative research it financially supports.

In anticipation of the dinner, the young faculty member reaches out to the chair of the committee that will be making the decision on the award. During their one-on-one meeting, they plan to discuss her research and what it is that she plans to speak about at the dinner. During the meeting, however, the funder begins to tell the professor about his personal connection to cancer within his family. "Cancer, now that’s something I know about. It took the lives of both of my parents. It is really a horrible monster that just runs through a person’s body, destroying whatever it finds in its path. It is great that there are scientists like you who are finding the cure—an antidote—to such a vicious disease. I think it would be really convincing to the committee to talk about how you’re helping people win the battle and to beat this foe. One day we’ll eliminate cancer!”

After her meeting, she sits down to outline her presentation and is presented with the challenge ahead of her. She knows that her choice to embrace the chair’s mischaracterization of cancer will likely give her an advantage in persuading the committee to help advance her research programme, but likely at the cost of misrepresenting the context and motivation for her research. It’s their funding, after all, that will help advance her research, not their understanding of the complexities of cancers and metal complexes. If she speaks too technically, however, she worries that she will lose the attention of her potential funders and miss out on an important opportunity.

Class No.	Class Title
16	Summary

Summary of content

In this last chapter, we will summarise all the aspects of *good chemistry* that we came across throughout the book. This is a challenge since, as we have seen, the professions that chemists can occupy, the realms in which they work, and the contexts in which the chemical expertise is applied, can vary quite largely. There is no standard way of doing good chemistry. The purpose of facing that challenge is to realise that none of the topics in this book is optional, luxury, or unimportant. In one or the other way, they all touch the daily activity of a chemical practitioner from time to time. This chapter is intended to illustrate the firm connections between methodology, professional integrity and social responsibility one more time. The examples – schedules of a busy day of selected chemical professions – may appear unrealistic due to their density of special scenarios accumulated in one day. Yet, all the chosen events pose challenges to the chemist's decision-making and judgment ability. Some are issues of critically reflecting methodological questions, others require a research or profession ethics approach, some are located at the intersection between chemical expertise (science, research, public service), society and environment, some touch all three categories at the same time. The reader is asked to transfer the quintessential conclusions from these cases to his or her real-life cases as chemistry students, academic scientists, researchers in private sector industry, or as chemists in public service.

Key Themes

Relevance of methodological clarity for professional integrity and social impact;
Professional integrity as good research practice and profession ethics;
The inevitable social impact of all chemical activity;
Taking responsibility = taking the right action;
Good chemistry as a discourse skill.

Learning Objectives:

After this summary, more than before, the reader will…

…see all the topics introduced in this book set into perspective in respective relevant contexts,

…understand why all three categories (methodology, research ethics, social implications) have their justification in a book on *Good Chemistry*.

…be able to apply the acquired knowledge of this book in the own particular research field and professional niche,

…apply all the insights from this course in order to contribute with his/her expertise to a sustainable and beneficial progress of science and technology, thus fulfilling the social responsibility as a chemist.

Course of progress

Step	Task	est. time
1	Warm-up reflection: Why nanoscience?	10 min.
2	Video lecture, part 1: Short overview of nanotechnology	30 min.
3	Reading assignment: Overview of "Nanoethics" (Grunwald 2012)	15 min.
4	Video lecture, part 2: The Nanopil project	15 min.
5	Further reading: The Nanopil project (Lucivero)	20 min.
6	Video lecture, part 3: Course summary	13 min.
7	Final reflection and discussion	20 min.
8	Quiz	5 min.