Chemical space: mathematical, computational and ethical questions arising from its historical unfolding

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Chemical space, understood as all known chemicals and reactions, is central not only because it constitutes the raw material of the discipline, but because it encodes patterns that shed light on the future of chemistry. In this talk I will discuss the evolution of the chemical space from 1800 up to the result of an ongoing research programme on processing electronic repositories of information with mathematical and computational tools. Chemical space has been expanded at an exponential rate with doubling times of 16 is marked by three statistical regimes on the production of chemicals with sharp 1860 and 1980. Interestingly, despite its rapid growth, chemical space has been, with the passage of time, more and more concentrated on the deep exploration of some of its those where organic chemistry lies. The expansion space leads to several questions, some are of computational nature and others of ethical tone. Mathematical and computational questions include the maximum size of the space, the conditions to increase its expansion rate and the historical nature of the ontology of chemistry. Social questions touch upon the institutional structures of chemistry accounting for the historical evolution and whether it is possible to tune them. Ethical questions are related to the kind of space we should aim at, for the sake of knowledge and of our presence on the Earth planet.