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Chemistry space—time☆

David A. Winkler[a,b,c,*]

[a] CSIRO Manufacturing, Bag 10, Clayton South 3169, Australia
[b] Monash Institute of Pharmaceutical Sciences, 390 Royal Parade, Parkville 3052, Australia
[c] Latrobe Institute for Molecular Science, Bundoora, Australia

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Abstract As Einstein identified so clearly, space and time are intimately related. We discuss the relationship between time and Euclidean space using spectroscopic and radioastronomical studies of interstellar chemistry as an example. Given the finite speed of light, we are clearly studying chemical reactions occurring tens of thousands of years ago that may elucidate the primordial chemistry of this planet several billion years ago. We also explore space of a different kind — chemical space, with many more dimensions than the four we associate as space—time. Vast chemical spaces also need very efficient (computational) methods for their exploration to overcome this 'curse of dimensionality'. We discuss methods by which the time to explore these new spaces can be very substantially reduced, opening the discovery useful new materials that are the key to our future.

Contents

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* Correspondence to: CSIRO Manufacturing, Bag 10, Clayton South 3169, Australia.
E-mail address: dave.winkler@csiro.au

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I wasted time, and now doth time waste me;
For now hath time made me his numbering clock;
My thoughts are minutes. — William Shakespeare

The relationship between space and time

''People like us, who believe in physics, know that the distinction between past, present, and future is only a stubbornly persistent illusion.'' Albert Einstein

Most physical scientists are aware of the intimate relationship between space and time. Einstein quantified and clarified this relationship in the theories of General and Special Relativity. Space—time is a mathematical model that unites space and time into a single interwoven continuum. It combines space and time into a single manifold called Minkowski space, as opposed to the commonly experienced Euclidian space (Fig. 1).

In cosmology, the concept of space—time combines space and time to a single abstract universe. Mathematically it is a manifold consisting of ''events'' which are described by some type of coordinate system. Typically three spatial dimensions (length, width, height), and one temporal dimension (time) are required.

Figure 1 Albert Einstein.

General and Special Relativity shows that space, time, and gravity are interlinked, and that gravity can warp space and distort time. The consequence of large spaces and the finite speed of light is long times. Astronomical observation necessitates seeing things far away and long ago.

Here we discuss the relationship between chemistry, time, and two kinds of 'space', interstellar (Euclidean) space, and chemical or materials space. In interstellar space we will discover primordial chemistry that is the key to our past, and in materials space we will discover new chemistry that is the key to our future.

Interstellar space, chemistry, and relationship to time

The Universe is approximately 13.5 billion years old, evolving steadily since the Big Bang. It is a very dynamic space with many very unusual non-equilibrium systems within it. Interstellar dust and gas clouds are the birthplaces of new stars, and are also where very interesting primordial chemistry occurs. Several of these interstellar gas clouds are in our Milky Way galaxy, and have been the source of intense spectroscopic analysis. Infrared (vibrational) and in particular, microwave (rotational) spectroscopy, have been invaluable for identifying the types of molecules and chemistry that occur within these clouds. These methods can also be useful for identifying the amount (column density) of small molecules present, the temperature, velocity, and magnetic fields (Brown et al., 1980a) present in the clouds. Molecular line radioastronomy has generated much information on the chemistry that occurs within interstellar clouds (Kroto, 1980) (Fig. 2).

The two most interesting and accessible molecular clouds in our galaxy are Sagittarius B2 (Sgr B2) near the galactic centre, and the Orion Nebula (M42) on an outer spiral arm of the galaxy. Sagittarius B2 is a giant molecular cloud of gas and dust that is located about 120 parsecs (390 light years (ly)) from the centre of the Milky Way and 27,000 ly from earth. It is the largest molecular cloud near the centre, ~45 parsecs (150 ly) diameter, and mass ~3 million solar masses. The mean hydrogen density in the cloud is 3000 atoms per cm^3, ~20—40 times denser than typical molecular clouds (Fig. 3).

The Orion nebula (M42) is located at a distance of 1344 ± 20 light years from the Earth and is the closest region of massive star formation to Earth. The M42 nebula is estimated to be 24 light years across. It has a mass of ~2000 solar masses.

Molecule densities are very low (10^6 hydrogen molecules/cm^3 in very dense clouds) with average kinetic temperatures 10—100 K, suggesting mean free paths of between 10^9 and 10^{15} cm. Time between collisions (10^4—10^{10} s) is of the order of relaxation times for