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ARTICLES:

"A clear magnetic light" - can metaphors help with scientific models in ESP? The case of gadolinium

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1. Introduction

Although metaphor has been identified and used as a figure of speech since the time of Aristotle at least, its cognitive importance has only recently been fully recognized with the cognitive theory of conceptual metaphors pioneered by Lakoff and Johnson:"The essence of metaphor is understanding and experiencing one kind of thing in terms of another" (1980: 5). Conceptual metaphors are reflected in set phrases and idioms at a linguistic level. Lakoff and Johnson conceive them as primarily rooted in embodied experience (1999: 44-59). For convenience sake, conceptual metaphors will be written in capital letters in this article and their linguistic counterparts in italics. HAPPY IS UP/SAD IS DOWN, for example, with instantiations such as *cheer up*, *ups and downs*, *to feel down*, *to be downhearted*, etc..., derives from the fact that lying down is often caused by tiredness or sickness, whereas the upright position is characterised by energy and movement. But Lakoff and Johnson also acknowledge that conceptual metaphors may also be influenced by culture. Examples such as *it's a waste of time*, *a time saving device*, *try to gain time*, etc..., can be related to TIME IS MONEY, and seem typical of our western civilization, but might not make much sense among traditional societies in Oceania or Africa. All conceptual metaphors operate by creating "a cross-domain mapping in the conceptual system" (Lakoff, 1973:203), i.e. by transferring the logic of a metaphorical source domain onto a target domain that is to be characterised.

The cognitive view of metaphors has been adopted for this study because it is based on a mapping process which is particularly coherent with the analogical transfer method often used in scientific theory (Hesse, 1966, King, 1991, Cowan et al., 1994, Montuschi, 2000, Gentner et al., 2001). Models in science can be broadly

defined as "simplified representations" (Crease, 1999) consisting in a transfer of shapes or structures from one domain to another (Black, 1962). Niels Bohr's representation of the atom as a miniature solar system is a typical historical example of how a better known domain (Newtonian mechanics) may be used to understand a less well-known one (sub-atomic particles).[1] The use of models dates back to the astronomical maps of the Greeks, but the development of computer calculating power has opened up a host of new possibilities for modelling and simulation, so that the important role played by models in scientific discoveries is now commonly acknowledged (Magnani et al, 1998).

Models and metaphors are relevant to the field of English for Specific Purposes (ESP) in a number of different ways. Most English teachers in science and technology departments are quite comfortable with metaphors, but find dealing with scientific models a daunting prospect, especially if they are fraught with equations. However, as models are becoming an essential channel of professional communication in modern experimental sciences as well as in information technology, they cannot be overlooked altogether. One solution may require resorting to an "expert informant" , i.e. a specialist of the domain who can provide explanations. If no such person is available, however, the similar mechanisms underlying models and metaphors prompt the question: can our knowledge of metaphor help us to understand scientific models, or at least to make sense of them in such a way that we can grasp the role they play in scientific communication? Given the exploratory character of the questions asked, a case study approach seems appropriate in order to explore their relevance in one scientific field before generalising to experimental sciences as a whole .

2. Materials and methods

The metaphors and models analysed in this study are taken from a review article on the use of gadolinium ions in Magnetic Resonance Imaging (MRI) published in *Chemical Reviews*, entitled: "Gadolinium chelates as MRI contrast agents: Structure, Dynamics, and Applications" (Caravan et al., 1999), and hereafter referred to as CR. This article summarizes the state of the art in MRI research for medical diagnostic applications at the end of the 1990s. MRI scans are now widely applied as a help for medical diagnosis because, unlike conventional radiography and computed tomographic imaging (CT) which use potentially harmful X-rays, it is a non-invasive procedure. The principle of the scans consists in using the magnetic properties of stable (non-radioactive) nuclei. Patients are placed in a tunnel-like tube generating a very strong magnetic field. Suitable pulses of radio-waves are then broadcast, which disturbs the magnetic properties of the hydrogen protons contained in the water molecules of our body. The time they take to return to equilibrium (the so-called relaxation rate) is monitored, and transformed into images via a computer. In order to enhance the pictures obtained, contrast agents may be used, the most popular being gadolinium, a “clear magnetic light” (CR:

[1]It is worth noting that Bohr's model is still being used in undergraduate classes for pedagogical purposes, although it has been outdated ever since Schrödinger's equations replaced Newtonian mechanics at a sub-atomic scale.

2293). Gadolinium ions have the property of enabling neighbouring hydrogen protons to relax faster, therefore enhancing the relaxation rate contrast between the tissues absorbing gadolinium, and the rest. Gadolinium ions are potentially toxic, but can be easily and safely trapped by chemical molecules called ligands to form gadolinium complexes.

The field of MRI studies was chosen for two reasons. First of all the complexity of the issue at stake, i.e. characterising through simple images and theories the effects of gadolinium ions in the macro-environment of billions of interacting molecules, implies an intensive use of models. Secondly, it has the advantage of being more inclusive, in as much as, besides its main grounding in physical chemistry, it makes use of different scientific fields: crystallography to determine the structure of molecules, coordination chemistry to synthesize new gadolinium complexes, mathematics to solve differential equations for relaxation theory, pharmacology to test *in vivo* compatibility and medicine to develop new applications for clinical diagnosis. This interdisciplinary scope offsets one of the limits of the case study approach, implying that the tentative conclusions reached may be generalised to a wider range of scientific fields.

Now that the field of MRI scans and contrast agents has been introduced, we can come back to the initial question asked: can conceptual metaphors help us make sense of scientific models? In order to answer it, we must first identify the types of models used in CR and their functions, then the conceptual metaphors found and the parts they play, before looking for interactions between models and metaphors.

3. Models: typology and functions

Let us first look at the types of models found in the CR article. Black[2] (1962) distinguishes between scale models (three dimensional miniatures or magnified versions of some material object), and theoretical models which are based on an identity of structure between two different fields and make an intensive use of mathematics. This typology is still relevant today, and comprehensive enough to include visual and mathematical as well as verbal models, which fits in well with the CR article.

Scale models are the easiest to recognize. They appear either with a tri-dimensional shape, or as a two-dimensional developed chemical formula. Let us take the example of gadolinium-DTPA, a chemical complex commonly used in medical MRI (see appendix n°1). In the developed chemical formula the atoms are represented by their acronym in the periodic table, and the chemical bonds by dashes (see appendix n°1 again). On the other hand, the three-dimensional model features each atom as a roughly spherical ball and each chemical bond as a link (in the displayed compact model links are embedded in atoms). On the whole, 147 developed chemical formulae appear in the CR article and 43 three-dimensional

[2] His influence was acknowledged by Johnson (1987) and Lakoff (1993), along with that of other philosophers of science such as Hesse and Boyd.

models, using up 13 pages out of 59, almost one quarter of the space. The distribution of scale models is not homogeneous throughout the article, however. On the one hand they are widely used to illustrate molecular special geometry in the parts entitled “Solution and Solid State Structure” and “Physical Properties of Small Molecule Gadolinium Complexes”. On the other, they are almost completely absent from the mathematical part, which sums up relaxation theory, and the clinical applications at the end (see appendix n°2). The origin of the three-dimensional models dates back to the beginning of quantum mechanics and to one of its basic postulates, the Pauli principle, which restricts the number of electrons occupying the same region in space. One of the consequences of this principle is that interpenetration is prevented in the regions occupied by the electrons around two atoms, except in case of a chemical bond (i.e. two atoms sharing a couple of electrons) where these regions can have a slight overlap defining the bonding zone. This accounts for the representation of atoms as impenetrable hard balls.

How can such a model help us to understand the theory of MRI relaxation contrast agents? We must remember that contrast agents work by helping water protons to revert to equilibrium more rapidly. The relaxing power of gadolinium in a given chemical complex depends, among other things, on the rotation movement of the complex, as well as the movements of the surrounding water molecules. This emphasizes the importance of being able to describe molecular movements. For that purpose a common (and sometimes rough) approximation consists in representing all contrast agents as spheres, whatever their actual shapes: “Water molecules and the Gd(III) complex are often treated as hard spheres” (CR: 2325). The molecular rotation movements are then much more easily set into equations. This is the case in figure 45 (cf. appendix 2), where the gadolinium-based contrast agent MS325 is represented as a small ball binding to an albumin cell in the shape of a bigger sphere: "The agent is shown schematically as consisting of two parts: a circular gadolinium chelate and a bullet-shaped protein-binding moiety." (C p. 2341) The example of figure 45 thus illustrates clearly how scale models aim at reproducing an original schematically, suppressing certain features, and emphasizing others.

While a scale model (of a molecule, for example) always has an important visual component, theoretical models are much more general and seek to reproduce a structure. In theoretical models, the intuition of an analogy between a real field and a mathematical structure is quantified through applicable mathematical formulae, although the price paid is some degree of simplification. The importance of mathematics in the CR article is directly expressed through 28 equations, two thirds of which being contained in the five pages summing up relaxation theory, and indirectly shown throughout the article by the use of 27 numerical tables which take up one sixth of the space (10 pages out of 59, see appendix n°2).

After this brief description of the range of models found, the question of their function can now be addressed. The models used in the CR article play a dual role: they enable us to visualise on the one hand, to explain and predict on the other. The

tri-dimensional scale model provides the best visual aid through its magnified version of the geometrical structure of the molecule: the links created by the chemical bonds, and their angles, the relative positions of the different atoms in the molecule.

While three-dimensional scaled molecules alone can function as a visual help, all models can be used to explain and predict (Hesse 1966: 157-177). In fact, explanation and prediction can be viewed as mirror images of the same process. On the one hand biological behaviour can be deduced from chemical properties through prediction, but on the other hand chemical properties can also be induced from biological observations, and this provides an explanation. The tri-dimensional model of DTPA, for example, can provide a visual account of how a gadolinium ion can be trapped (see appendix 1). A DTPA molecule can take different shapes, according to the way the different atoms move around their chemical bonds. The negatively charged nitrogen and oxygen atoms of a DTPA molecule are attracted by a positively charged gadolinium ion (coloured in red in the middle), and tend to move around their chemical bonds so as to trap, or complex, this metallic ion.

In the case of theoretical models, predictive ability is an essential element of validity, so that they develop in a continual exchange between experiments and mathematical formalism. For example this is shown quite clearly with the in vivo stability problem (cf appendix n°4). As free gadolinium is a potentially toxic metal ion, contrast agents can only be inoculated in vivo if the complexing molecules can trap gadolinium efficiently. One of the ways of solving this problem is to start from the fundamental thermodynamic properties of a molecule, and predict its in vivo behaviour. The simplest model consists in using the thermodynamic stability constant KGdL, defined by equation 7 (cf. appendix n°4). This model can be refined by taking the acidity of the liquid into account, and defining a new conditional stability constant K*ML, calculated according to equation 8. Then, in order to check experimentally if the thermodynamic stability predictions still apply in vivo, the contrast agent studied is injected into mice, and the quantity of free gadolinium ions found in the skeletons is measured seven days later. If neighbouring values for the conditional stability constant match neighbouring doses of gadolinium found in the skeletons, the prediction is verified, and the model validated. This is in fact not the case here, as the authors' provisional conclusion acknowledges: "Thus it is clear that thermodynamics, i.e. the gadolinium stability constant alone, is not sufficient to explain in vivo stability trends." (C. p 1315). The model must be further extended, taking into account the affinity of the complexing molecule for other metallic ions, as well as for gadolinium. This in turn leads to new equations, new tests, etc, until experimental results are in good agreement with predictions based on thermodynamic properties.

This brief overview of some of the models used in the field of MRI is an illustration of how widely they are used, a popularity which can be explained both by the need to visualize molecular interaction, and the time gained in projecting

successfully the structure of a well-known domain onto a less well-known one. Let us now turn to the metaphors contained in the CR article.

4. Metaphors: typology and functions

The metaphors contained in the CR article were identified by the present author, which made it possible to use conceptual metaphor theory in that task, and also to match the identification criteria with the purpose of this article (see Low 1999: 49). If we remember that the point of view adopted is that of a layperson trying to grasp MRI models through the metaphor she selects, it does not really matter if some of the metaphors are overlooked: if they are opaque to her, they would not be of any use in order to help understand models. The metaphors selected were then checked with an expert informant to offset the subjective character of unilateral identification, and make sure that all the phrases selected were indeed metaphorical (see Low 1999:49 again).

184 metaphors were found in the 59 pages and 24,689 words of the CR article, which amounts to an average of a metaphor every 134 words, and a little over three metaphors per page. Globally, metaphors are only slightly outnumbered by visual models (184 versus 190), and share with them an uneven distribution throughout the article (see appendix n°2). Predictably, the parts using most metaphors are the least technical ones: the introduction (one metaphor in every 48 words), and the clinical applications at the end (one metaphor in every 83 words). On the other hand, the parts containing the fewest metaphors focus either on mathematics ("Relaxation Theory", with a rate of one metaphor out of every 575 words) or on physics ("Physical properties of Small Molecule Gadolinium Complexes", featuring only one metaphor in every 668 words). Other results, however, are more surprising at first sight. The part describing the physical structure of chemical molecules ("Solution and Solid State Structure") is above average for its content of metaphors (one in every 95 words) as well as scale models (two-thirds of the visual models in half of the pages). On second thoughts, though, this fits in well with a strong need for visualisation in a part describing molecular geometry.

After this brief quantitative overview, let us now turn to the conceptual metaphors found, and how the analogical mapping they are based on functions, projecting characteristics of a concrete domain (the source, in cognitive semantics terms) onto a more abstract one (the target). In the CR article, metaphorical targets are mostly either chemical molecules or on scientific theory, in a direct link with the contents (see appendix n°6). Source domains for molecules are borrowed either from the construction industry, or from personification. The source domain of civil engineering allows one to conceive intramolecular connections over atoms or groups of atoms as bridges: *bridging ligand* (CR: 2311*), bridged trimer* (CR: 2303), *ethelene bridges* (CR: 2311). The most frequent source by far, however, is the human body. It has the same origin as visual models, which represent molecules as balls: gadolinium is portrayed as *a little hydrophylic ball* (CR: 2295). Through metonymy (a ball has the same shape as a human head) and synecdoche (the head stands for the whole person), we come to the end result A MOLECULE IS A

PERSON. This personification is nowhere openly acknowledged but functions throughout the article as an overarching subconscious conceptual metaphor leaving clues at the linguistic level of metaphorical expressions. This is reminiscent to the way Turner and Fauconnier (1995: 188) analyse the desk-top metaphor as an interface between human users and home computers: "The user is not manipulating this computer interface by means of an elaborate conscious analogy, but as an integrated form with its own coherent uses and properties". A mapping of the metaphor links different parts of the body with various parts of a molecule: the "*face"* represents the front of a molecule: *the phosphinate oxygen face of the molecule* (CR: 2304), *the twist angles between the faces* (CR: 2306). "*Arms"* project onto peripheral moving parts*: acetate arms* (CR: 2302, 2312, 2313*), hydroxypropyl arm* (CR: 2313). "B*ackbones"* are likened to central parts (*backbone of the ligand* (CR: 2300), *terminal backbone nitrogens* (CR: 2311)). These metaphorical uses of *arm* and *backbone* seem to be conventional rather than creative, which can be checked easily in *Chemical Abstracts*, a database containing the article abstracts of the most well-known chemical journals. The phrase *pendant arm* appears 406 times in *Chemical Abstracts* and *lysine backbone* 101 times. This conventional character has even led to lexicalisation, since *arm* has become the established way of referring to "linear chains attached to a central unit" in a molecule, and *backbone* to "the main chain of atoms", according to the American Heritage Dictionaries.

These words do not seem to have any non-figurative synonym (just as there is no non-figurative way of referring to the leg of a table), but, beyond filling a gap in the lexis, they also play an important role as "theory constitutive" metaphors, as argued by Boyd:

> There exists an important class of metaphors which play a role in the development and articulation of theories in relatively mature sciences. Their function is a sort of catachresis - that is, they are used to introduce theoretical terminology where none previously existed. (1993: 482)

The official adoption of "*arm"* and "*backbone"* by the discipline of physical chemistry, rather than, say, "lungs" or "kidneys", is constrained by the subject of the article: understanding the use of gadolinium involves primarily making sense of molecular interactions, which map onto body movements, and the body parts being able to move, i.e. limbs and backbone. This can be shown as follows. From the premises that persons have arms and backbones (including elbows, wrists, knuckles and vertebrae), we can infer that joints allow us to take special positions and to move. This non-metaphorical entailment related to the human body is projected onto a metaphorical one in the target domain of coordination chemistry: molecular arms and backbones help to account for special atom positions within the complexing molecule (i.e. molecular geometry), as well as for molecular movements (e.g. trapping a gadolinium ion to form a chemical complex). Selected fixed geometries are described according to different criteria: they can take into account either the global geometrical structure of the molecule ("*wrapping*

isomers" CR: 2310,11,12,13), as from a distant view, or only part of it ("*capped plane*" CR: 2303, "*capping position*" CR: 2301, 4, 7) as in a close-up. This duality of a partial versus a global geometry is also relevant in a dynamic approach, separate limb movements mapping onto specific local changes of positions of the atoms, and global body motion onto full intra-molecular dynamics (cf. table 1 below[3]).

PERSON	MOLECULE
premises:	parallel premises:
1) Persons have faces, arms and backbones	1') Molecules have"*faces*","*arms*", and "*backbones*" "*phosphinate oxygen face*" (CR: 2304) "*twist angles between the faces*" (CR: 2306) "*acetate arms*"(CR: 2312),"*hydroxypropyl arm*" (CR: 2313),"*phosphonate arm*"(CR: 2313),"*pendant arm*" (CR: 2314) "*lysine backbone*" (CR: 2336), "*diclohexyltriamine backbone*" (CR: 2297), "*backbone of the ligand*" (CR: 2300), "*terminal backbone nitrogens* " (CR: 2301)
non metaphorical entailments:	metaphorical entailments:
2) our limbs and backbone allow us to take special positions	2') molecular arms and backbones form peculiar atomic geometries "capping positions" (CR: 2301), "capped planes" (CR: 2303), wrapping isomers (CR: 2310)
3) our limbs and backbone allow us to move	3') molecular "*arms*" and "*backbones"* help to account for molecular movements "*shuffling* of coordinated acetates" (CR: 2310), "*flip* of the backbone ethylenes"(CR: 2310, 11), "*tickling* "(CR: 2293), "*intricate danse*" (CR: 2295)
4) our limbs and backbones allow us to perform actions with our whole bodies	4') molecular *"arms"* and *"backbones"* help to account for organised intermolecular movement, i.e. actions "small iron particles can *function as T1 agents*" (CR: 2295), "The texaphyrin ring… *acts as* a monoanion" (CR: 2308), "donor atom" (CR: 2300)

Table 1

[3] In this article, metaphorical inferences have been represented in tables rather than with arrows, following Rohrer (1995, 1997) so that entailments can be clearly highlighted.

This first entailment could be summed up as MOLECULAR POSITIONS ARE BODILY POSITIONS. It can be extended to: MOLECULAR MOVEMENTS ARE BODILY MOVEMENTS. This is already exemplified in the introduction to the article, in which a global view on gadolinium is adopted. It is introduced as "this potentially toxic metal ion which floats among the water molecules, *tickling* them magnetically" (CR: 2293)

This tickling corresponds to the crucial interaction of the gadolinium electrons with the nuclear magnets of the water protons. Their coupling is minute in comparison with the violent direct collisions of a gadolinium complex with a water molecule, which justifies the use of "*tickling*". In the case of dysprosium Dy (III), a neighbouring lanthanide ion, the coupling becomes so fast that it has no effect on the nuclear magnets, as expressed by this aesthetic, even exotic appraisal: "In the *intricate danse* that gives rise to relaxivity, water protons hardly *feel* the effect of ions such as Dy(III), *much like a leaf near the incredibly rapid wings of a humming-bird*." (CR: 2295)[4]. In other words the stimulus becomes too rapid to be felt. After the introduction, in the description of molecular structures, the target domain focuses on what happens inside molecular complexes, with either disorderly movements: "the *shuffling* of coordinated acetates" (CR: 2310), or rapid to-ing and fro-ing: "a *flip* of the backbone ethylenes ..."(CR: 2310-11). Molecules are then tackled more globally in the rest of the article. They are pictured as able to perform actions (thanks to movements), and the first two entailments are subsumed under a more general third one: MOLECULAR ACTIONS ARE BODILY ACTIONS, with instantiations such as: “small iron particles can *function as T1 agents*” (CR: 2295), “The texaphyrin ring… *acts as* a monoanion” (CR: 2308), or “*donor atom*” (CR: 2300). In the part dealing with clinical applications, molecules are even endowed with human-like perception, and even judgment:
“MRI agents which *sense* their biochemical environment“ (CR: 2348)
“MRI enzymes which *sense* the presence of particular enzymes” (CR: 2348).
“Lanthanides tend to favour high coordination numbers in aqueous media” (CR: 2296)

The conceptual metaphor A MOLECULE IS A PERSON therefore seems to be the most consistent way of conceptualising molecules in the CR article. This seems paradoxical at first sight, since scientific writing is widely considered as being impersonal, as acknowledged for instance in *A Grammar of Contemporary English* (Quirk et al., 1972: 808): “The passive is generally more commonly used in informative than in imaginative writing, notably in the objective non-personal style of scientific articles and news items.” This frequent use of passives is correlated in scientific discourse with a strong tendency to nominalize processes into objects, in order to measure them more easily. The first sentence in the second paragraph of the CR article exemplifies both trends: “The successful *penetration* of gadolinium chelates into radiologic practice and medicine as a whole *can be measured* in many

[4]This simile can be considered as a figurative extension of the MOLECULAR MOVEMENTS ARE BODILY MOVEMENTS entailment, as interacting bodies are not human persons, but instead leaves and hummingbirds.

ways." (CR: 2293) This gives the overall picture of an impersonal world populated with objects.

It would be unfair, however, to stop there. As experimental scientists choose to disappear behind passives in the research articles they write, they also endow objects and abstract notions alike with human-like skills (see Banks 1994: 90-103, Fries 2005: 235-236). In the CR article, figures, data and studies are capable of ostention: "table 11 *shows*…" (CR: 2318), "this result *highlights* a key-point" (CR: 2316). They can also produce descriptions: "These equations *describe* relaxation as a function of magnetic field" (CR: 2321), and even make demonstrations on their own: "Neutron diffraction studies… *demonstrate* that this angle can be quite varied…" (CR: 2322). These personifications can therefore pragmatically be considered as a sort of hedges (see Lakoff 1972), one of the many ways used by scientists to disguise their presence in scientific research articles and avoid potential controversy with their peers. This clearly shows that personification has a part to play in modern scientific prose, and that the conceptual metaphor A MOLECULE IS A PERSON is by no means as incongruous as it seems at first sight.

Let us now come back to the cognitive function of this metaphor. According to Lakoff and Johnson, personifications:

> "allow us to make sense of phenomena in the world in human terms - terms that we can understand on the basis of our own motivations, goals, actions, and characteristics." (1980:34).

When gadolinium is presented as "*tickling*" water molecules(CR: 2393), the humorous personification contained in "*tickling*" enables the reader to picture the incredibly rapid movements (nanoseconds, or even less) of minute molecules (a few angströms wide) by transferring them to a human scale. It also implies that the interaction between gadolinium and water is superficial, fast, and does not produce any lasting change.

Another dimension of personification according to cognitive semantics is embodiment, with the claim that the experience we have of our bodies in space can be mapped onto more abstract domains (see in particular Johnson, 1987), especially thanks to conceptual metaphor. Rohrer (2005) surveys no less than 12 dimensions of the term embodiment in cognitive science. In the fourth dimension, called "perspective", he points out that "we routinely project the canonical orientations of our embodiment onto the objects of the world" (2005: 9). This explains the use of prepositions such as "in front of" or "at the back of". It also motivates many of the names chosen to describe landscapes:

> "In English we can speak metaphorically about features of the landscape in terms of the body, such as *the face of a mountain, the mouth of a river, the foothills,* and so on… In other words we understand features of the landscape metaphorically, using our bodies as the grounding frame of reference." (2005: 5)

Mutatis mutandis, the adoption of "*arms*", "*backbones"* and "*faces"* in chemical parlance is also due to a projection of bodily experience onto molecular structure. The personification of molecules in the CR article therefore has a double cognitive role: enabling us to describe phenomena at an infinitesimal scale, and to make sense of their spatial geometry.

In the CR article, the most popular target domain for metaphors, after molecules, is theories, which comes as no surprise for a survey dealing with fairly abstract models. Two major conceptual metaphors are used: THEORIES ARE JOURNEYS, and THEORIES ARE MINING. The THEORIES ARE JOURNEYS metaphor foregrounds an ongoing process. Problems regarding discoveries are mapped onto a horizontal plane, with obstacles to be overcome: "*One hurdle that remains* in these systems is the coordination of endogenous anions..." (C p. 2334). In this context, the obstacles which runners have to jump over in a race are projected onto the difficulty of designing safe small molecule contrast agents which do not lose part of their relaxive power when coordinating with anions such as phosphate or bicarbonate. Framing the journey as a race of hurdles implies that the only permissible way of overcoming obstacles is to jump over them: "*Once the chemist makes the mental leap*, however difficult it is, that this exchange labile metal ion forms essentially inert complexes, then the chelate can be viewed as an intact drug molecule." (CR: 2295). Here, the obstacle is not experimental, as in the case of molecule design, but theoretical: how does gadolinium complex? As this positive metal ion has only a weak bond with each of the negatively charged atoms it is linked to, an easy escape from these bonds is to be expected in traditional coordination chemistry, creating potential health hazards. Surprisingly, it happens to be safely trapped in some complexing molecules. Each of the two plausible scenarios accounting for the complexation of gadolinium is represented as a plot of ground, and their incompatibility as a ditch, or a river. Leaping over the gap from one field to the next one maps onto the intellectual risk involved in giving up the safe old field of coordination chemistry, and venturing into risky gadolinium pharmacology. Although very general in scope, the conceptual metaphor THEORIES ARE JOURNEYS seems nevertheless appropriate for a review article in which the expert is taking the medical readers by the hand to guide them through difficult chemical theory and call their attention to some of the issues at stake in order to achieve the end of better care for patients.

While the THEORIES ARE JOURNEYS metaphor foregrounds an ongoing process whose different stages are mapped onto theory, THEORIES ARE MINING frames problems regarding scientific discovery on a vertical plane, with precious ore awaiting excavation. This conceptual metaphor is common in English, with instantiations such as "*he was a gold-mine of ideas*", "*now we have to refine those ideas*", "*What I like about his book is that he brought some deeply buried ideas to light*". In the history of mining, however, the work of geologists and that of chemists which refined the ore into elements are interestingly intertwined, which provides a more subject-specific motivation for this metaphor. The opening sentence in the introduction of the CR article reads: "Gadolinium, an obscure

lanthanide element *buried in the middle of the periodic table*, has in the course of a decade become common place in medical diagnostic." (2293). The whole article is thus framed within the THEORIES ARE MINING metaphor, and all the efforts made to save gadolinium from centuries of neglect highlighted. All the hard work reviewed, however, may not suffice, as the following sentence, taken from the end of the article, shows: "However, as noted by the authors, *layers of targeting and pharmacokinetic challenges remain* before receptor-based MRI agents can be used in vivo." (CR: 2341). This sentence stresses the main challenge MRI biomedical researchers are currently faced with: targeting contrast agents to particular organs or specific tissues, while avoiding any harmful side-effects for the patients. The THEORIES ARE MINING metaphor therefore highlights the efforts necessary to come to a "deeper" understanding of the subject.

The THEORIES ARE MINING and THEORIES ARE JOURNEYS metaphors draw on different spatial dimensions, and are construing different problems in different frames (“digging” versus “hurdling”). And yet they both have the same function: they help us to visualise abstract problems: difficulties are pictured in terms of "*layers of targeting and pharmacokinetic challenges*" to be cleared away, or as "*hurdles*" to be overcome by "*mental leaps*". The digging or travelling frames do not seem to have any direct cognitive impact here, as they do not contribute to a new understanding of the difficulties encountered. However, they draw the lay readers’ attention to some of the major theoretical issues at stake, therefore enabling them to gain time.

5. Practical applications for ESP

At the end of this brief survey of models and metaphors in a scientific review article, let us come back to the initial question asked: can metaphors help the ESP teacher understand models, when reading scientific articles? Black (1962) and Hesse (1966) have successfully used traditional metaphor theory to account for the explanatory and predictive properties of models. The analysis of models and metaphors in the CR article exemplifies this point of view: both models and conceptual metaphors on gadolinium complexes work by creating a mapping between different domains: atoms and balls, molecules and persons, theories and journeys, etc... This common mechanism can prompt us to consider models as a special type of metaphor (Crease, 2000). One can further argue that models are a special type of conceptual metaphors, because they are more precise about what topographies and topologies they preserve as they map knowledge from the source domain into the target domain. Specifically, models preserve topologies that have predictive power, typically in the sense of a mathematical prediction. Metaphors preserve these, but to a much lesser extent. In the case of gadolinium complexes, all the models can be seen as instantiations of the underlying conceptual metaphor A MOLECULE IS A BALL.

The question of whether metaphors can help in the understanding of models seems therefore justified, from a theoretical point of view. But does it have practical use? If we remember that both metaphors and models work by setting up analogical

mappings between a well-known domain and a less well-known field on the one hand, and that theoretical models make an intensive use of abstraction on the other hand, it follows that metaphors may rightly be used as a shortcut through equations, tables of figures, diagrams, etc... But does it in fact work? In other words, are they a suitable tool to help us grasp the issues at stake, even if we don't understand all the mathematical subtleties involved?

In the CR article, metaphors give us useful insights into theory. In the introduction, for example, gadolinium is described as "*this clear odorless 'magnetic light'* " (C p. 2293). The use of inverted commas in the text clearly indicates that the phrase '*magnetic light'* should not be taken literally, and earmarks it as metaphorical. One of the properties of light is to reveal contrasts coming from differences in properties. These contrasts can come either from various parts of the object considered, or from discrepancies between the object and its environment. This power to reveal differences in properties is mapped onto an ability to create different relaxation rates thanks to the presence or absence of gadolinium. In MRI diagnoses, contrasts appear when various tissues relax at different rates, and these relaxing rates depend in turn on the quantity of contrast agents absorbed (here gadolinium complexes). The greater the absorption, the quicker the relaxation. Just as the observation of different light contrasts enables us to constitute a picture, MRI images are based on the more or less intense colouring of different relaxation zones. The *'magnetic light'* metaphor thus enables us to grasp the function of gadolinium directly, without delving into molecule structures or relaxation theory. The fact that it appears in the opening page of the article is also worth noting: by providing a quick overview of the state of the art in gadolinium studies, it allows radiologists and other members of the medical profession to skip to the medical applications at the end of the article with a general understanding of the issues at stake in mind, if they wish to. The context in which "*magnetic light*" is placed thus enables us to say that it may indeed be used as a heuristic tool to facilitate the understanding of relaxation models, as it is pragmatically cutting short through theoretical paraphernalia.

Unfortunately, all the metaphorical expressions used by Caravan et al. do not work this way. If we go back to the exchange dynamics of DTPA molecules in a solution, for example (cf. appendix n°5), the metaphorical expressions "*backbone ethylenes*" and "*acetate arms*" can be quite confusing to the lay reader. The ethylenes are situated on the outside of the molecule, and drawn in an elongated shape suggesting an arm, whereas the acetates are represented with curved lines reminiscent of a bent back. In this case the metaphor is intended to focus the reader's attention on a particular aspect of molecular shape change, which proves misleading for the layperson.

This pair of contrasting examples shows quite clearly that an understanding of models gained solely through metaphors may prove relevant. A metaphor such as GADOLINIUM IS MAGNETIC LIGHT has a source domain rooted in bodily experience, so that no specialized knowledge is required for its understanding. Yet

it sums up the scientific argument at stake efficiently, thereby giving the ESP teacher a general grasp of the subject, and allowing her to gain time. However, the counter-example of backbone ethylenes and acetate arms also shows that common sense and everyday experience cannot be assumed to be totally reliable. These mixed results stem from the fact that although different theories of models and conceptual metaphor hang together, because they are motivated by similar concerns about pattern preservation, yet they function to preserve patterns at different levels of generality, which can create misunderstandings.

6. Conclusion:

To conclude, a comparative analysis of models and metaphors (in the case of gadolinium complexes) reveals differences in their functions. Conceptual metaphors map bodily experience onto the molecular world, but they also throw light on the difficulties of the research process, whereas models allow visualisation, explanation and prediction. These discrepancies nevertheless hide a common core: models can also be considered as surface instantiations of the conceptual metaphor A MOLECULE IS A SPHERE, on which the personification of molecules is based. Tying up models with conceptual metaphors also has practical implications as far as the comprehension of scientific English is concerned. Seeing metaphors as a help in order to understand scientific models in fact follows the same line as using models in order to understand the world. We take a familiar domain (metaphors), and apply it to another less well-known domain, i.e. scientific models, in order to understand them. This approach can allow ESP teachers to cut short through equations and theoretical discussions, and grasp the scientific issues at stake in a global way, which can certainly save time. However, just as the insights gained through models must be in agreement with experimental results, vicarious understanding of models through metaphors should always be checked with an expert informant.

Acknowledgments:

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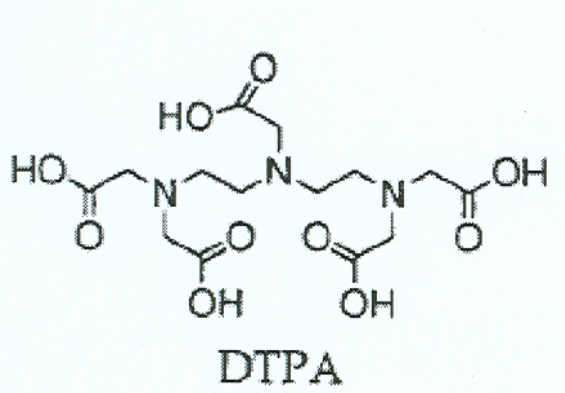
APPENDIX n°1 :
scale models in chemistry



Developed chemical formula of DTPA

Three-dimensional model of DTPA

APPENDIX n°2

Contents of the CR article	**Metaphors**	**Scale models**	**Numerical tables**	Mathematical equations	Chemical equations
I Introduction (pp2293-95)	**26**	**0**	**0**	0	0
II Solution and Solid State Structures (pp 2295-2320)	**111**	**128**	**11**	8	5
III Relaxation theory (pp 2320-2325)	**6**	**1**	**1**	19	0
IV Physical Properties of Small Molecule Gadolinium Complexes (pp 2326-2336)	**4**	**41**	**8**	1	0
V Macromolecular Conjugates (pp 2336-2341)	**14**	**9**	**4**	0	0
VI Relaxivity of Non-Covalently Bound Adducts of Gadolinium (III) Complexes (pp 2341-2344)	**6**	**9**	**2**	0	0
VII & VIII General Physicochemical Properties and Safety (pp 2344-2346)	**3**	**0**	**1**	0	0
IX Applications (pp 2346-2348)	**13**	**2**	**0**	0	0
X Conclusion (p 2348)	**1**	**0**	**0**	0	0
Total	**184**	**190**	**27**	28	33

APPENDIX n° 3

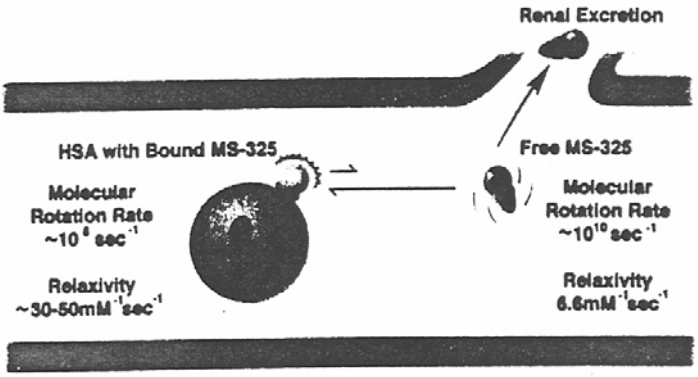


Figure 45. RIME mechanism of action for MS-325. The agent is shown schematically as consisting of two parts: a circular gadolinium chelate and a bullet-shaped protein-binding moiety. Within the bloodstream, MS-325 binds, on average, to one of many available sites on HSA. The bound form is in equilibrium with a small amount of the free form which is renally excreted steadily over time. The bound form of MS-325 has greatly enhanced relaxivity by virtue of its slower molecular tumbling rate.

APPENDIX n° 4

macokinetics, protein binding, elimination, and safety. Equilibria between gadolinium(III) and other competing endogenous metals and anions can potentially contribute to the dissociation of gadolinium(III) from the complex, an event which removes the critical magnetic core of the drug. By design, the magnitude of the thermodynamic stability constant K_{GdL}, defined in eq 7,[120] is large for all of the clinically viable

$$M + L = ML \qquad K_{ML} = \frac{[ML]}{[M][L]} \qquad (7)$$

contrast agents, ranging from $10^{16.85}$ for [Gd(DTPA-BMA)] to $10^{25.6}$ for [Gd(DOTA)] (Table 10). Clearly, the equilibrium in eq 7 lies heavily to the side of the complex, GdL, and little, if any, free metal is present at equilibrium under conditions where eq 7 is valid.

The coordination chemist will appreciate the fact that protons will compete for the ligand L as the pH is lowered; this competition must be taken into account if one is to understand the solution equilibria at physiological pH. This is critical for the multidentate, multiprotic ligands which are being discussed in this review. Given the protonation constants of the ligands and the formal stability constant K_{ML}, the conditional (or pH dependent) stability constant K^*_{ML} can be calculated using eq 8. The conditional stability constant K^*_{ML} is often used to compare the relative thermodynamic stability of different chelates at pH 7.4. Table 10 also reports the conditional stability constants for the series of clinically relevant contrast agents as well as $[Gd(EDTA)(H_2O)_n]^-$.

$$K^*_{ML} = \frac{K_{ML}}{(1 + K_1[H^+] + K_1K_2[H^+]^2 + \ldots + K_1K_2K_n[H^+]^n)} \qquad (8)$$

where K_1, K_2, K_3, ... K_n are the stepwise protonation constants of the ligand.

Given that there is a difference in the relative thermodynamic stability of these compounds at physiological pH, how do these data correlate with observed in vivo results, particularly the deposition of dissociated gadolinium(III) in the skeleton? To investigate this question, Wedeking et al.[121] have measured the %ID (initial dose)/gram found in the femur at 7 days postinjection (mouse) for a series of clinically relevant extracellular contrast agents (Table 10) with similar pharmacokinetic and elimination characteristics. $[Gd(EDTA)(H_2O)_n]^-$ was not an approved contrast agent, but was included for comparison purposes.

When comparing the complex stability in Table 10 to the amount of gadolinium(III) found in the rodent skeleton at 7 days, it is immediately striking that while thermodynamic (K_{ML}) and conditional stability constants (K^*_{ML}) values for $[Gd(EDTA)(H_2O)_n]^-$ and $[Gd(DTPA\text{-}BMA)(H_2O)]$ are relatively similar (for example, K^*_{GdL} = 14.9 and 14.7, respectively, for L = EDTA and L = DTPA-BMA), the amount of Gd(III) deposited in the mouse at 7 days is rather significant (~0.8%ID/gram) for $[Gd(EDTA)(H_2O)_n]^-$ and small for $[Gd(DTPA\text{-}BMA)(H_2O)]$ (~0.03%ID/gram).[121] Likewise, the amount of Gd(III) found in the bone for $[Gd(DO3A)(H_2O)_n]$ is surprisingly small given the rather low conditional stability constant. Thus, it is clear that thermodynamics, i.e., the gadolinium(III) stability constant alone, is not sufficient to explain in vivo stability trends.

Cacheris et al. evaluated the relationship between thermodynamics and toxicity for a series of gadolinium(III) complexes and also concluded thermodynamic stability of the Gd(III) complexes in itself was insufficient to correlate observed acute toxicity (not bone deposition) for a series of Gd-153 labeled DTPA derivatives examined in rodents. In their study, the authors assumed that acute toxicity was related to the dissociation of gadolinium(III). Consideration of the relative affinity of the ligands for Gd^{3+} as well as biologically relevant cations such as Ca^{2+}, Zn^{2+}, and Cu^{2+} led the authors to propose the use of a "selectivity" factor, log K_{sel}, to accommodate the biological data. Table 10 shows the observed LD_{50} in mice,[122-125] stability constants for the ligands with Gd(III), Ca(II), Cu(II), and Zn(II),[28,47,51,126-130] as well as a selectivity factor, log K_{sel}, which was calculated using eq 9. This factor takes into account the ligand

APPENDIX n° 5

Table 8. Kinetic Data for Rearrangements in Ln(III) Complexes

complex	$\Delta G^{\ddagger}$ (kJ mol^{-1})	$\Delta H^{\ddagger}$ (kJ mol^{-1})	$\Delta S^{\ddagger}$ (J mol^{-1} K^{-1})	k_{ex} (s^{-1})	dynamic process[a]	ref
Pr(DTPA)	56.5(3.6)	35.2(2.0)	−71.4(5.8)	265 (278 K)	A	92
Eu(DTPA)	55.4(4.6)	38.5(2.4)	−56.8(7.0)	360 (278 K)	A	92
Yb(DTPA)	49.4(10)	37.0(5.0)	−41.7(16)	4300 (278 K)	A	92
Nd(DTPA-BPA)	53(1)			350 (283 K)	A	80
Eu(DTPA-dienH$^+$)	57.5(0.3)					41
La(DTPA-BPA)	71(1)	47(8)	−84(25)	0.7 (283 K)	B	80
Lu(DTPA-BPA)	67(1)	42(8)	−88(20)	2.4 (283 K)	B	80
La(DTPA-BGLUCA)	66	34	−116	2.7 (283 K)	B	100
La(DTPA-BENGALAA)	65	37	−100	0.7 (283 K)	B	100
Lu(DOTA)	65.9(1.2)	100.5(0.6)	116(2)	18 (298 K)	C	45
Yb(DOTA)	65.9(1.0)	82(12)	52(39)		C	93
La(DOTA)	60.7(1.2)	59.4(0.8)	−4.6(3.3)	23 (278 K)	D	103
La(DOTP)	101(11)				D	105
Lu(TETA)	63.7(7.5)	71.7(5.3)	27(8)	7 (278 K)	E	114

[a] A: exchange between wrapping isomers. B: racemization of terminal backbone nitrogens. C: enantiomerization. D: ring inversion. E: exchange between dodecahedral conformations of TETA.

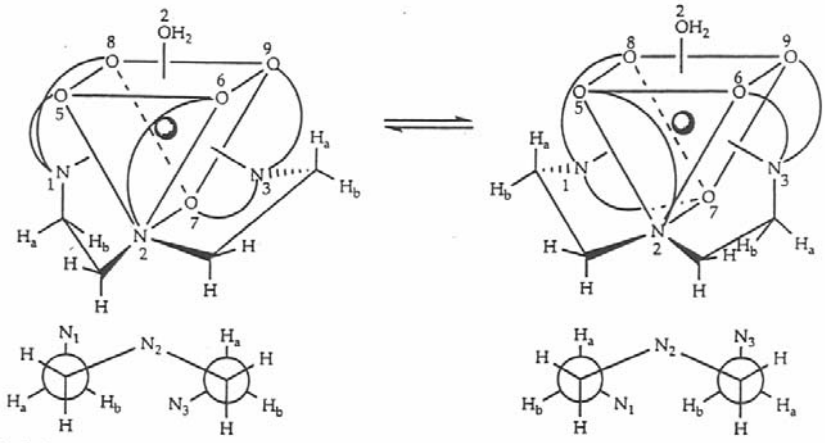


Figure 28. Rapid exchange interconversion between wrapping isomers of Ln(DTPA) results in a psuedo mirror plane, reducing the number of observed proton resonances by half.

The major feature of the exchange process involves the shuffling of coordinated acetates accompanied by a flip of the backbone ethylenes between staggered conformations (see Figure 28). This results in a change in the helicity of the complex and leads to the equilibration of two of the acetate arms, which alternate coordination of position 7, and converts axial ethylenediamine protons to equatorial.

APPENDIX n° 6 :

Metaphors found in the Chemical Review (CR) article

A MOLECULE IS A CIVIL ENGINEERING STRUCTURE
a *bridging* bidentate group occupying the ninth coordination site of a neighbouring metal center (2297)
bridging carboxylates (2301)
carboxylate *bridged* dimmer (2302)
bridged trimer (2303)
a bidentate carboxylate group which *bridged* from the first complex (2303)
bridging carboxylate groups (2305)
ethylene *bridges*(2311) +1
bridging ligands (2311)
a *scaffold* for the attachment of various chelates (2339)

A MOLECULE IS A LIVING BEING
magnetic *core* (2315) *"core"* molecules (2338) acid *core* (2339)
stems from (2294)+1
nitrogen *mustard* (2295)
to *muck up* our DNA (2295)
the *tether* between amide groups (2311°

A MOLECULE IS A PERSON

MOLECULAR PARTS ARE BODILY PARTS
backbone 10
backbone ethylene 2
the *backbone* of the ligand (2300)
the diethylenetriamine *backbone* 2
terminal *backbone* nitrogens 3, central *backbone* nitrogen 2
lysine *backbone* (2336), dextran *backbone* (2340)
acetate *arms* 9, hydroxypropyl *arm* 3
pendant *arm* 3, phosphonate *arm* 2
the phosphinate oxygen *face* of the molecule(2304)
the twist angles between the *faces* (2306)

MOLECULAR POSITIONS ARE BODILY POSITIONS
capping position(s) 6
monocapped arrangement (2301) *monocapped* plane (2306)
capped planes 3 (2302) 2 (2303)
a water molecule *capping* the phosphinate oxygen face of the molecule(2304)
wrapping isomers 4
the ligand is then able to *wrap* round the metal center (2299)
ligands incapable of *wrapping* around the metal center (2311)

the *shuffling* of coordinated acetates accompanied by a *flip* of the backbone ethylenes (2310)
exchange by *flip* of the backbone ethylenes… and *shuffling* of the donor acetates (2311)

MOLECULAR MOVEMENTS ARE BODILY MOVEMENTS
this potentially toxic metal ion which swiftly *floats* among the water molecules, *tickling* them magnetically (2293)
the successful *penetration* of gadolinium(III) chelates into radiologic practice (2293)
the unique magnetic properties of the gadolinium (III) ion *placed* it right in the middle of a revolutionary development (2293)

MOLECULAR ACTIONS ARE BODILY ACTIONS
there is nothing a good nucleophile or electrophile can *attack* (2295)
a good T1 agent would not significantly *affect* the bulk magnetic susceptibility of the tissue compartment in which it is localised (2295)
small iron particles can *function* as T1 agents (2295)
the texaphyrin ring …*acts as* a monoanion (2308)
it is not uncommon for a ligand to *form* isostructural chelates (2308)
these isomers *exchange* very slowly (2311)
a blood pool agent which…*exhibits* enhanced reaxivity (2342)
this compound was designed to *targe*t tumour cells… (2343)
encapsulated chelates do not *show* the same r1 enhancement as… (2343)
prolonged *trapping* in the liver (2346)

MOLECULAR ROLES ARE HUMAN ROLES
donor atom(s) 10
neutral *donors* 2, Amide *donors*, *Donor* groups (2317), ligand *donor* set (2336)
a ligand carboxylate *donor* (2297)
oxygen *donor* atom 4, oxygen *donors* (2305)
a bridging carboxylate *donor*, amide oxygen *donors* (2300)
the 4 *donor* phosphinate oxygens (2304)
donor acetate (2311) acetate *donor* (2336)
parent ligands (2318)
a *key-role* (2316)

MOLECULAR FEELING IS HUMAN FEELING
In the *intricate dance* that gives rise to relaxivity, water protons *hardly feel* the effects of ions such as Dy(III), much like a leaf near the incredibly rapid wings of a hummingbird (2297)
MRI agents which *sense* their biochemical environment (2348)
MRI enzymes which *sense* the presence of particular enzymes (2348)

MOLECULAR JUDGMENT IS HUMAN JUDGMENT
lanthanides tend to *favour* high coordination numbers in aqueous media (2296)

AN OBJECT/PROCESS IS A PERSON:

- an object is capable of ostention as well as a person:
table 11 *shows* …the data *show*...(2318) Table 28 *shows*… (2345)
several examples have *shown* (2314) the data *show* (2318) an accumulated body of literature has *shown* (2316) chelates do not *show* (2343) A field that *shows* a great deal of promise ... the results *show*...(2344) Clinical trials repeatedly *showed* no significant difference… (2346)
an accumulated body of literature has *shown* (2316)…
this result *highlights* a key-point (2316)
a blood pool agent which... *exhibits* (2342)

- an object is capable of description as well as a person:
table 1 *lists* (2293) Table 11 *lists* (2316)
papers have appeared which *detail*... (2317)
these equations *describe* (2321)
these equations *describe* relaxation as a function of magnetic field (2321)

- an object is capable of logical reasoning as well as a person:
iron particles... *lead to* a much larger increase 2294)+2
the solution structures... *agree with* their solid state structures (2316)
examination of table 10 *reveals* (2316)
absorbtion spectroscopy… also *suggested*… (2316)
the studies of Wedeking and others *contradict* this prediction (2316)
the accumulated body of literature which *has established* (2316)
data accumulated over the past ten years *indicate*… (2320)
neutron diffraction studies… *demonstrate*… (2322)
the simulation of vanadyl EPR lines shapes *can distinguish between* isotropic an anisotropic motion(3223)
the tables *will explicitly note* the chemical structure (2336)

THEORIES ARE MINING
the LIS effect has an r-3 dependance from which structural information about the chelate *can be extracted*, eq 5 (2309)

CHEMISTRY IS MINING
the metal ion *is buried* in the cage (2295)
with EXSY, chemical exchange *is probed* using a standard NOESY pulse sequence (2309)
layers of targeting and pharmacokinetic challenges remain before receptor-based MRI agents can be used in vivo (2341)

THEORIES ARE JOURNEYS
once the chemist *makes the mental leap* (2295)
structural characterisation *is the first step* in understanding… (2295)
one *hurdle that remains* in these systems… (2334)

GADOLINIUM IS MAGNETIC LIGHT
'magnetic light' (2293)
the ability *to image* low concentration receptors (2336)
blood pool *imaging* (2336)
the goal of *imaging* receptors using MRI… (2336)
new applications involve faster *imaging* drug injection to obtain images of arteries or of blood flow to the heart (2346)
prolonging blood half-life and *imaging window* (2346)
early interest in *tumour imaging* (2347)
MRI *images* (2347)
the *detailed images* of biological functions (2348)

Miscellaneous:
activation parameters... are expected to *reflect* the data (2311)
the perceived clinical properties of this agent *mirror* the biochemical consequences of its chemical structure (2346)
a *trade-off* (2324)
this *translates to*… (2327)
phosphate *buffer* (2334) *buffered* aqueous solution (2339)
"magic bullet" targeting (2346)
Just a tuning-fork (2348)

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ABSTRACT

"A clear magnetic light" - can metaphors help with scientific models in ESP? The case of gadolinium

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Key-words
ESP, mapping, metaphor, model, science

Most English teachers in science and technology deal more easily with metaphors than with scientific models, especially if they are fraught with equations or figures. And yet, both models and metaphors are based on a transfer of meaning from one domain to another. The main question addressed in this article is whether metaphors can be used to help in making sense of models. To answer this question, an in-depth analysis of the models and conceptual metaphors found in a review article on gadolinium was carried out in comparison with a corpus of six "hot" articles published by the American Chemical Society. The results show that metaphors can indeed be used as a short-cut through theory, helping English teachers to grasp the main issues at stake. However, this vicarious knowledge always needs to be checked with an expert informant, just as the insights gained through models must be in agreement with experimental results.

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