

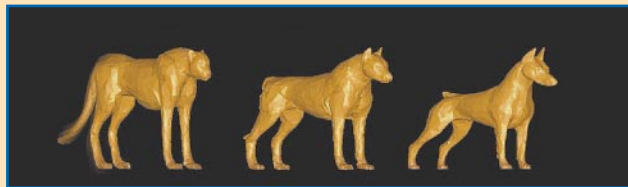
Cats, dogs and categories

Any child can tell a cat from a dog. But the difference has to be learned, and describing it is far from simple. Cats include cheetahs, lions and tabbies; dogs include Siberian huskies and dachshunds. How do we make the jump from recognizing a particular set of features to establishing a more general concept or category that will help us extrapolate to new situations?

Writing in last week's *Science* (291, 312–315; 2001), David J. Freedman and colleagues describe how they have explored this question by training monkeys to distinguish between 'catness' and 'dogness'. The authors used computer graphics to create blended images from a set of three dog and three cat images. An example of a cheetah, a Doberman and, in between, a blend of the two is

shown on the right. They then taught the monkeys to indicate, by releasing a lever, whether a sample image was of the same type as a test cat or a test dog. Monkeys, it turns out, are good at learning this distinction: even when the image was 60% cat and 40% dog, the monkeys reliably reported that it was like a cat. Furthermore, monkeys were not simply memorizing specific blends of cats and dogs as belonging to one category, because new blends were tested during the experiment.

To find out how these categories are represented in the brain, the authors recorded neural activity in the lateral prefrontal cortex — an area of the frontal lobes previously implicated in guiding complex behaviours — while the monkeys performed the task. Surprisingly, they found category



information represented at the level of single neurons. That is, regardless of whether the image was 60%, 80% or 100% dog, individual neurons responded in a similar way; but they responded differently for 60%, 80% or 100% cat.

Obviously, these category representations were the result of training — neurons in a monkey's lateral prefrontal cortex probably don't care about 'dogness' under normal circumstances. Indeed, the authors

went on to train one of their monkeys on a new, more abstract categorization of the same images, and showed that neurons no longer distinguished cats and dogs as they did previously, but now coded for the new categories. How these representations come to be formed rapidly and reversibly in this part of the brain is not going to be easy to answer. But it is clearly closely related to how we learn to categorize our world into meaningful concepts.

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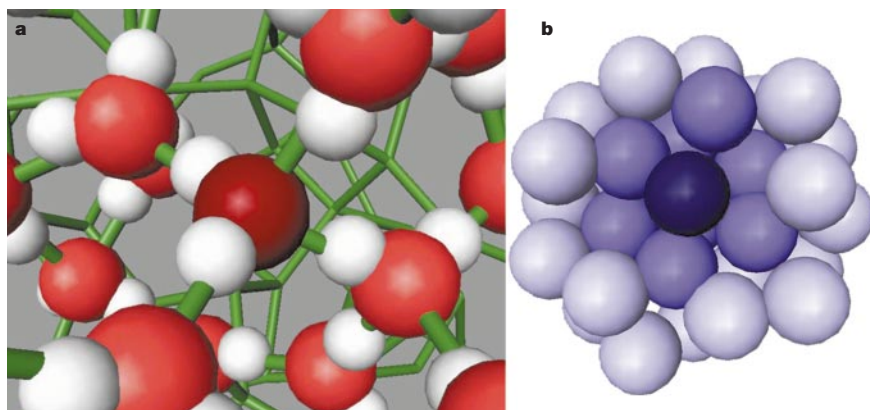


Figure 1 Molecular structure in liquids. **a**, In water, molecules typically form hydrogen bonds (green bars) with four neighbours, and the liquid displays an open, loosely packed, structure. Hydrogen atoms are shown in white, oxygen atoms are red, and the central oxygen atom is dark red. Only the molecules within the first two neighbouring shells are shown, but all the bonds are indicated. **b**, In a simple atomic liquid, the packing is much more dense. The first two neighbouring shells of the dark-blue central atom are shown, and the atoms in front of the plane of the central atom have been removed, for clarity.

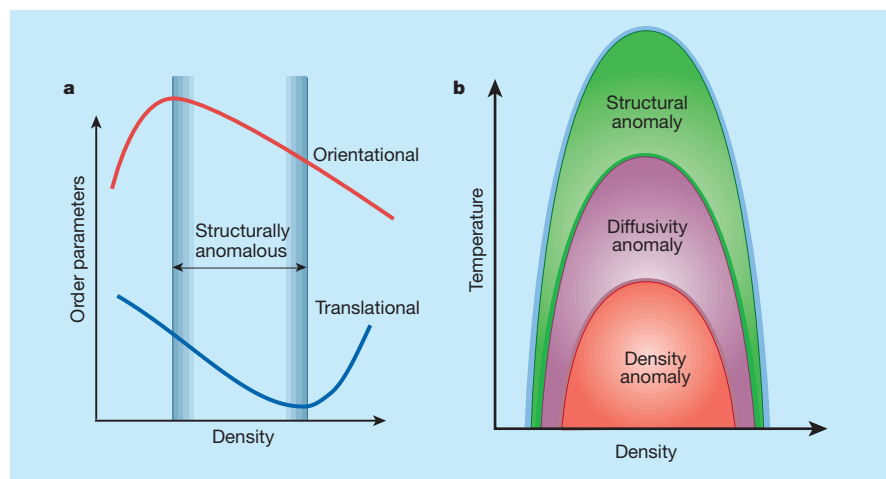


Figure 2 A possible link between structural order and anomalous behaviour in liquid water. **a**, The typical density dependence of orientational and translational order parameters. Errington and Debenedetti¹ identify a ‘structurally anomalous’ region, bounded at low densities by an orientational-order maximum, and at high densities by a translational-order minimum. **b**, In the density–temperature phase diagram, the ‘structurally anomalous’ region forms a dome, which encompasses the regions of dynamic (diffusivity) and thermodynamic (density) anomalies.

Whereas repulsions determine this short-range order in normal liquids², the architects of local structure in water are hydrogen bonds. These bonds require pairs of molecules not only to be optimally separated, but also to have a specific orientation. In the most energetically favoured structure, each molecule has four hydrogen-bonded neighbours that sit at the corners of a regular tetrahedron (Fig. 1a), in contrast to about twelve neighbours in an atomic liquid (Fig. 1b). Water molecules are therefore less densely packed, and water possesses a far greater degree of local ‘orientational’ order than normal liquids. Qualitatively, many of water’s peculiarities can be understood from this observation alone³.

Errington and Debenedetti shed new light on the relationship between the structure of water and its anomalous behaviour

by focusing on global aspects of structural change. They define two order parameters. The first quantifies translational order: how neighbours of a molecule are distributed, on average, in their distance from the molecule. The second parameter quantifies orientational order: the extent to which neighbouring molecules are at specific angles with respect to each other. In normal liquids, both translational and orientational order increase with density. In water, however, for a range of densities and temperatures, both translational and orientational order decrease when density increases, because compression leads to a disruption of the network of hydrogen bonds. Errington and Debenedetti identify this as their ‘structurally anomalous’ region. At a fixed temperature, this region is bounded by an orientational-order maximum at the low-

Daedalus

David Jones

David Jones, author of the Daedalus column, is indisposed.

density end, and by a translational-order minimum at the high-density end (Fig. 2a). The structurally anomalous region forms a ‘dome’ in the density–temperature diagram (Fig. 2b).

Errington and Debenedetti show that the regions of peculiar diffusivity and density are nested like Russian dolls within the region of structural anomaly (Fig. 2b). So liquid water appears to have a hierarchy of anomalies: the structural anomalies occur over the broadest range of temperatures and densities, within which are found both the diffusivity and density anomalies.

Another curious pattern emerges when the values of the orientational and translational order parameters, at various densities and temperatures, are plotted against each other in a ‘parametric plot’. All available pairs of values fall to one side of a boundary line and, remarkably, points corresponding to the structurally anomalous region all appear to fall on the boundary itself (see Fig. 5 on page 320). Because the boundary is a one-dimensional line, the translational order and orientational order are strongly coupled within the structurally anomalous region.

Errington and Debenedetti’s observations raise interesting questions and open a new line of investigation. The characterization of structural anomaly in terms of the strong coupling between translational order and orientational order may help to identify precise conditions necessary for anomalous behaviour. But at present it isn’t clear why this observed relationship and the nested pattern of structural, dynamic and thermodynamic anomalies hold, and whether we should expect to find them in other liquids as well.

It will be useful to apply the present analysis to other network-forming liquids that display structural and other anomalies — silicon and silica, which form tetrahedral networks in the liquid and solid states, are obvious candidates. If these results prove robust, they will have established a significant link between anomalous behaviour and the strongly correlated changes of translational and orientational order in network-forming liquids.

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2. Chandler, D., Weeks, J. D. & Andersen, H. C. *Science* **220**, 787–794 (1983).
3. Ball, P. *H₂O: A Biography of Water* (Weidenfeld and Nicolson, London, 1999).