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Tracking transition states through bond orders

The most direct approach to the understanding of reaction mechanisms is by examining potential energy surfaces in detail. A few stationary points, viz. the minima characterizing the reactants, products and potential intermediates and saddle points connecting them in an idealized cross-section, are specially important. Within transition state theory, the information about these points is just about everything one may wish to know about the course of the reaction. Minima are directly accessible to experimental investigations. But transition states are elusive. Kinetic experiments can yield activation energies, but not any precise details of other properties of the transition state.

Chemists are not put off by the difficulties associated with precise characterization of transition state structures. They invariably visualize reactions in terms of making, breaking or rearrangement of a few bonds. The 'action' is assumed to be localized in a small fragment even in a complex substrate. The simplified notions serve their purpose; after all, many reactions are used in predictable ways to make new compounds. But can the 'arrowpushing' approach be placed on a firmer footing? Can theory help?

Bond order, in spite of being only a computable property, is a concept which has found widespread acceptance among chemists. It is intuitively reasonable besides being intimately related to measurable quantities like bond lengths and bond energies. The latter are relatively difficult to calculate using quantum chemical methods for large molecules. On the other hand, sensible bond orders can be obtained even with fairly simple computational methods. Variations in bond orders have been suggested to be useful indicators of the changes oc-

curing during the course of a description for many simple reactions in the last few years. The inflexions noted in the bond orders have also been suggested to correlate well with the location of transition states. A detailed analysis with more complex examples is now provided (Maity *et al.*, page 343).

The approach employed by the authors is not going to replace conventional interpretations based on potential energy surfaces. The work is not meant in that spirit either. Just as orbital energy changes along the reaction coordinate can provide additional insights when interpreted with care, the methodology proposed based on bond orders represents another framework for understanding reactions. The language would also be familiar to nontheoreticians.

Animal welfare

Shivi, a king in the Mahabharatha, once gave protection to a dove which was being pursued by a hawk. The hawk demanded that the dove be handed over, but Shivi refused to do so, saying that he was obliged to protect it. The hawk then protested that this would mean starvation for him, and that Shivi himself would be responsible for the death of yet another living being in his attempt to save one life. In response, Shivi drew out his sword and proceeded to cut off his own flesh to offer it to the hawk and at the same time save the dove. The conflict portrayed here between the kind act of the king to save the dove and the cruelty that it would otherwise inflict on the hawk is almost eternal and haunts us in our ways of dealing with animals. The lesson conveyed, however, is simple and effective: if we do have the will, a little sacrifice on our part can achieve a lot for the welfare of animals.

King Shivi we may not be, but we could at least occasionally spare a thought for our fellow animals, exploited mercilessly ever since the dawn of our 'civilization' so that we may live a little longer, a little better. This is the theme of the special section on animal welfare in this issue of *Current Science*, a series of articles which attempt to present various aspects of our use of non-human animals.

The way we treat animals might largely rest on the contemporary philosophical strength of our civilization and on the extent of our realization that we, the humans, have a duty to think and worry about the welfare of animals just as we do about ourselves. Anindya Sinha (page 296) writes about these duties of the human race and reviews some of the old and new ideas that have guided our ethics of animal exploitation. This is followed by an appeal (page 301) by the noted primatologist Jane Goodall to initiate a dialogue on how noninvasively and painlessly animals can be used, if at all they must be, in the course of experimentation and education. She also identifies the responsibilities of the institutions of higher learning and the role they can play in minimizing the ill treatment that animals are often subjected to.

The tender relationship the farmers have with their herds of cattle, goat and sheep in Indian villages probably forms an exemplary way to incorporate the lesson from Shivi's legend. These farmers often take care of their domestic animals with extreme kindness, the kind that they show only to their own children, but at the same time they also subject them to hard work for their livelihood. It is not unusual to find, in our villages, the farmers tenderly touching their animals, hand-feeding the cattle late at night, and grooming them as they are given rest amidst the heavy working schedule. Does this physical touch elicit any healthy

response from the cattle? Natalie Waran in her article (page 303) on human-animal interactions explores the evidence that these do indeed greatly affect the psychological disposition of animals towards humans, their own survival, and possibly even productivity. Unfortunately, following the introduction of the western mechanized system of dairy management in India, the way cattle are treated has been changing: from a family companion to a mere productive unit. This dichotomy between the east and the west in their treatment of animals is the basis of the article by Madhusudan Katti (page 305), who outlines the actual realities that characterize human-animal conflict in most situations.

Natalie Waran, in yet another article (page 308), discusses various modifications of the immediate environment of the captive animal which should be achieved in response to its physical, social and developmental

needs. The importance of both these approaches for the well-being of our otherwise exploited livestock cannot be overemphasized. Finally, N. Winskill *et al.* draw attention to a specific example of the devastation that our maltreatment of domesticated animals can wreak (page 310), with a paper on the behavioural abnormalities of stabled horses.

In today's difficult world, it is often quite easy to ignore whatever does not attract our direct attention. We may thus never give a thought to the hundreds of cows that produce our breakfast milk, nor remember the thousands of monkeys that have been sacrificed to produce one effective drug. At the other end of the spectrum, it may be impossible to change the ways in which the majority of our self-driven humanity thinks. There are, however, small steps that we can take so that the animals that we use can live life somewhat better, possibly a little

more painlessly. As Edmund Burke said: '... nobody makes a greater mistake than he who did nothing because he could only do a little ...'.

K. N. GANESHAIAH
ANINDYA SINHA

More on the NSU

The debate on the National Science University was closed with the publication of the final reports on the NSU in the 25 June issue of *Current Science*. However, we have received more correspondence, some of which appears in this issue. Future letters on this subject will be published only if new points that have not been stressed so far are made by correspondents.

P. B.