Defining hydrogen bond through IUPAC

During the four years from 2006 to 2009, SciFinder has added 44,262 papers containing the term 'hydrogen bond'. To be precise, these many papers were added between 26 December 2005 and 13 January 2010, when the searches were made. This amounts to about 30 papers a day, a few more than one every hour. Hence, it is surprising to find that most authors still feel uncertain about what a hydrogen bond is. There are numerous definitions and it appears that the only consensus till now is that there is no universally accepted definition for the hydrogen bond. Considering the enormous interest and following our suggestion, the International Union of Pure and Applied Chemistry (IUPAC) formed a task group with 14 experts to come up with a modern definition of the hydrogen bond. The task group was chaired by E. Arunan (Indian Institute of Science, Bangalore) and S. Scheiner (Utah State University, USA) was the co-chair. Along with them, G. R. Desiraju (Indian Institute of Science, Bangalore), R. A. Klein (University of Bonn, currently at Cambridge, UK) and J. Sadlej (University of Warsaw, Poland) formed the core-group. I. Alkorta (Instituto de Quimica Medica, Spain), D. C. Clary (University of Oxford, UK), R. H. Crabtree (Yale University, USA), J. J. Dannenberg (City University of New York, USA), P. Hobza (Academy of Sciences of the Czech Republic), H. G. Kjaergaard (University of Copenhagen, Denmark), A. C. Legon (University of Bristol, UK), B. Mennucci (University of Pisa, Italy) and D. J. Nesbitt (University of Colorado, USA) were also part of the task group. The task group organized a discussion meeting in Pisa during September 2005 in which 12 of the task group members and 12 other experts spoke on hydrogen bonding. Extensive discussions on all aspects of hydrogen bonding took place and a definition was proposed. This was deliberated at length through electronic-mail within the task group. A year later, in September 2006, the core-group met in Bangalore. There was a one-day discussion meeting where four core-group members and five other experts made presentations. Following this, the core group produced a recommendation for the definition of hydrogen bonding. This proposal now had a short definition that insisted on some evidence for bond formation. Six criteria were given which could be taken as evidence for hydrogen bond formation; six other characteristics were listed completing the recommendation. Several foot-notes were added for clarifications where necessary.

Following discussions within the task group and after considering the comments from numerous experts across the world, the recommendation was revised and submitted to the Physical and Biophysical Chemistry Division of IUPAC in 2007. The Division felt that a detailed manuscript should be produced which summarizes the history of hydrogen bond research and provides a rationale for the new definition. The task group produced a consolidated technical report which was submitted to IUPAC in January 2010. After an extensive review process by the Division, a technical report on defining the hydrogen bond and the recommendation on the definition of the hydrogen bond have been accepted for publication in Pure and Applied Chemistry in October 2010. The recommendation has appeared in the IUPAC website as a provisional recommendation and IUPAC will accept comments on this recommendation until 31 March 2011. It can be viewed at the following website: http://media.iupac.org/reports/provisional/abstract11/arunan_310311.html.

In addition, details of the task group activities can be found at the following websites: IUPAC: http://www.iupac.org/web/ins/2004-026-2-100; IISC: http://ipc.iisc.ernet.in/~arunan/iupac/

Anyone interested in hydrogen bonding is welcome to go through the task group recommendation and send comments during the review period. The report and recommendation are available from the author as well.

1. See http://ipc.iisc.ernet.in/~arunan/iupac/ for a compilation of definitions over the last century.