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Refereed Article

Ross D. King, Nathalie Marchand-Geneste, and Bjørn K. Alsberg:

A quantum mechanics based representation of molecules for machine inference

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Abstract: *The problem of representing molecular structure has been one of the most important in the development of applied inductive logic programming (ILP). We present a new relation method for representing structure based on ILP and quantum mechanics. We have previously developed a 3D electronic structure representation using quantum topology called StruQT. This is based on Richard Bader's quantum topological atoms in molecules (AIM) theory, where points (critical points) with zero gradients on the electron density field of the molecules are of central importance. These critical points are connected through a network of gradient paths that show strong correspondence with the traditional model of atoms and bonds in a molecule. This paper extends StruQT by making it relational, and so removes the need to align molecules when it is applied. We show how StruQT is encoded in Prolog and apply it to a series of 2-chloro dibenzofurans. The relational StruQT representation can be extended to represent any other field.*

Publication and review history

This work was first presented at the Machine Intelligence 18 Workshop, held on September 19-21, 2001 at the University of York, UK. Attendance at this workshop was based on invitations. Speakers at the workshop were invited to submit their articles for consideration in the forthcoming workshop volume. The subsequent publication and review history for the present article was as follows.

1. First versions *published* by Linköping University Electronic Press on in August - October, 2001 and permanently available at
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2. First version *accepted* after due refereeing and according to scientific journal standards by the Electronic Transactions on Artificial Intelligence (ETAI) on 21.9.2001. Authors were invited to revise their articles, if they so desired, based on comments by the reviewers.
3. Revised version *accepted* on 4.12.2001.
4. Revised version *published* by Linköping University Electronic Press on 28.2.2002 and permanently available at the same URL as mentioned above.
5. Revised version appears in Electronic Transactions on Artificial Intellligence, Volume 5 (2001), section B, pages 127–142. The section and the annual volume are made permanently available at
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6. Paper editions of the ETAI issue and the ETAI volume containing this artice *republished* by the Royal Swedish Academy of Sciences.

The review policy and the quality requirements for acceptance are documented at http://www.etaij.org/info/

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