The RTAM electronic bibliography, Version 17.0, on Relativistic Theory of Atoms and Molecules

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September 6, 2013

Abstract

The RTAM bibliography is freely available at *rtam.csc.fi* and the Version 17.0 of August 22, 2013 now contains 16566 items from the years 1916-2013. 'Production works' were systematically covered until 1999. Since the year 2000, mainly methodological papers were included. The methods and principles behind RTAM are described.

Keywords:
Relativistic effects, atomic calculations, molecular calculations.

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(75 words.) [Relativistic effects strongly influence the properties of heavier atoms and molecules. The RTAM bibliography is a collection of 16566 references on the topic, starting from Sommerfeld (1916).]

Relativistic Quantum Chemistry has become a fertile and large field, to the extent that it may occasionally be difficult to locate in the literature the items, relevant for further work. One modest tool may be the three books by the author, called Relativistic Theory of Atoms and Molecules I-III[1–3], covering papers in 1916-85, 1986-92 and 1993-99, respectively. An analysis by the topic was also provided, making the books a *bibliographie raisonnée*. The electronically searchable RTAM file *rtam.csc.fi* was made available in 1995 and has now gone through 16 previous editions. It covers the latter half of the three books, plus further post-1999 references. Until the year 1999 an attempt was made to include both methodological papers and 'production' articles. Since the year 2000 only the methods work, and applications of personal interest to the author were in principle included.

Most of the references were located by following the current literature in theoretical chemistry, inorganic chemistry, or chemical physics. Some further items were found through the ISI Web of Knowledge for the years 2000-12 by search terms 'relativistic OR Dirac'. The search was terminated in the summer of 2013. I apologise for any inadvertent omissions.

The search engine has the fields ANY, AUTHOR, TITLE, JOURNAL and YEAR, plus an AND/OR/AND+NOT command. For special letters, one can use '?' for a free letter and '*' for a free string. For instance, M?ller will recover Muller, Müller, Miller, Møller,.. but not Mueller. M*ller will include it. You may search for isolated words but not for strings. To look for Y-F Zhao, eliminating other Zhao:s, use AUTHOR Zhao AND AUTHOR Y-F. An efficient way to search for data on a given element, such as gold, is to combine a case-specific (so far two-letter) chemical symbol and a name: [case specific] TITLE Au OR TITLE gold.

The answers are given in BibTex format, making their use in manuscripts easy.

Including the material in the previous three books, the present RTAM data file contains 16566 items. Although the intellectual content of this source may not be much higher than the intellectual content of a telephone directory, the users' response has been positive.

Thanks are due to CSC (Centre for Scientific Computing, Espoo, Finland) and in particular Dr. Nino Runeberg for maintaining the RTAM service.

References

1. Pyykkö, P. *Relativistic Theory of Atoms and Molecules. A Bibliography 1916-1985*, *Lecture Notes in Chemistry*, Vol. 41, pages i–ix, 1–389, Berlin, 1986. Springer-Verlag.

2. Pyykkö, P. *Relativistic Theory of Atoms and Molecules. II*, *Lecture Notes in Chemistry*, Vol. 60, pages i–viii, 1–479, Berlin, 1993. Springer-Verlag.

3. Pyykkö, P. *Relativistic Theory of Atoms and Molecules. III*, *Lecture Notes in Chemistry*, Vol. 76, pages i–x, 1–354, Berlin, 2000. Springer-Verlag.