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### DESCRIPTION

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*Computational and Theoretical Chemistry* publishes high quality, original reports of significance in **computational** and theoretical **chemistry** including those that deal with problems of structure, properties, energetics, weak interactions, reaction mechanisms, catalysis, and reaction rates involving atoms, molecules, clusters, surfaces, and bulk matter. Reports on new algorithms and comprehensive assessments of existing ones, and applications to new types of problems are especially welcome. Manuscripts that apply standard methods to specific chemical problems and/or to specific molecules are appropriate if they report novel results for an important problem of high interest and/or if they are used to develop significant new insights.

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### AUDIENCE

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Chemical Physicists, Chemists, and Biochemists concerned with the application of theoretical methods for the resolution of practical chemical problems

### IMPACT FACTOR

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### ABSTRACTING AND INDEXING

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[1] J. van der Geer, J.A.J. Hanraads, R.A. Lupton, The art of writing a scientific article, *J. Sci. Commun.* 163 (2010) 51–59.

Reference to a book:

[2] W. Strunk Jr., E.B. White, *The Elements of Style*, fourth ed., Longman, New York, 2000.

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[3] G.R. Mettam, L.B. Adams, How to prepare an electronic version of your article, in: B.S. Jones, R.Z. Smith (Eds.), *Introduction to the Electronic Age*, E-Publishing Inc., New York, 2009, pp. 281–304.

Reference to a website:

[4] Cancer Research UK, Cancer statistics reports for the UK. <http://www.cancerresearchuk.org/aboutcancer/statistics/cancerstatsreport/>, 2003 (accessed 13 March 2003).

Reference to a dataset:

[dataset] [5] M. Oguro, S. Imahiro, S. Saito, T. Nakashizuka, Mortality data for Japanese oak wilt disease and surrounding forest compositions, *Mendeley Data*, v1, 2015. <https://doi.org/10.17632/xwj98nb39r.1>.

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