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WORKING PARTY ON STANDARDS FOR PRESENTATON OF DATA†

GUIDELINES FOR THE PUBLICATION OF RESEARCH IN EXPERIMENTAL ORGANIC CHEMISTRY

(Technical Report)

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Guidelines for the publication of research in experimental organic chemistry (Technical Report)

Abstract

Guidelines for the description of experimental procedures, for the characterization of compounds, and for presentation of derived physico-chemical quantities and mechanistic interpretation are formulated. These Guidelines are recommended as a minimum set for the publication of research in experimental organic chemistry.

A research paper in organic chemistry often contains one or more of the following features

- description of experimental procedures
- characterization of compounds
- derived physico-chemical quantities and mechanistic or other kind of interpretation

PROCEDURES

The experimental procedures should be published in adequate detail to enable another researcher to reproduce the experimental evidence. Well-known standard procedures and procedures which have been published in detail elsewhere and to which proper reference is given, constitute exceptions to this requirement.

The yield of preparative reactions should be stated as the range of yields actually obtained from the procedure in its developed form. Hazardous procedures and extreme toxicities of compounds (as far as known) should be clearly identified.

CHARACTERIZATION OF COMPOUNDS

Whenever possible, elemental analyses (C, H and *e.g.* N or S) should be provided for new compounds. However, the molecular formula may be determined from physical data, if evidence of purity is presented.

For each new compound at the end of a synthesis sequence there should be, in the light of its synthesis, explicit evidence and a convincing discussion of its *structural assignment* on the basis of *e.g.* COSY or other NMR data, X-ray (broadly to confirm to recommendations of the International Union of Crystallography) UV/Vis (wavelengths or frequencies and molar absorption coefficients) and IR data (including relative intensities: str, w, etc.)

Purity should appear from chromatography and melting point or boiling point.

When enantiomeric excess is claimed, sufficient supporting evidence should be presented.

Each major new compound should be identified by a systematic name at least once in a paper.

DERIVED QUANTITIES AND MECHANISTIC INTERPRETATION

The calculation, from primary experimental results, of quantities such as rate constants, as well as the derivation of a reaction mechanism are not always unambiguous. Therefore, it should be clearly stated how quantities have been calculated from the primary analytical data, what the experimental ranges and conditions are, and how large are the errors. In any case all quantities such as rate constants, NMR shifts, etc. should be accessible to the reader, even if subsequent steps in the analysis are straightforward. SI quantities, units and symbols should be used as far as reasonably possible.

The author of a *Preliminary Publication* should provide adequate description of the experimental methods and results. It is expected that such a publication will be followed by a full paper.