This article was downloaded by:

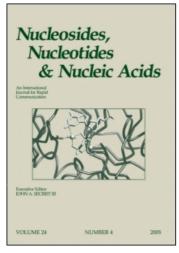
On: 27 January 2011

Access details: Access Details: Free Access

Publisher Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-

41 Mortimer Street, London W1T 3JH, UK



Nucleosides, Nucleotides and Nucleic Acids

Publication details, including instructions for authors and subscription information: http://www.informaworld.com/smpp/title~content=t713597286

Erratum

To cite this Article (1991) 'Erratum', Nucleosides, Nucleotides and Nucleic Acids, 10:4,911-912

To link to this Article: DOI: 10.1080/07328319108046670 URL: http://dx.doi.org/10.1080/07328319108046670

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.informaworld.com/terms-and-conditions-of-access.pdf

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

ERRATUM

The following additional material was provided by Dr. Wilson when it was discovered that it was inadvertently not included in the draft that was published (N & N, 9, 479).

FURTHER COMMENTS ON THE CONTRIBUTION OF EXOCYCLIC SUBSTITUENTS TO BASE-PAIR PROPELLER TWIST

C C Wilson

Neutron Science Division, ISIS Facility,
Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK.

Abstract

The arguments and results regarding base-pair propeller twisting calculated excluding the exocyclic base atoms are restated, updating the results given previously¹.

Introduction

In a recent paper¹, the propeller twists in a series of base-paired nucleic acid components were surveyed. It was found that the value of propeller twist was significantly affected by the exclusion of exocyclic base atoms from the calculations. The aim of this note is to amplify and clarify these previous results.

TABLE 1 - Selected average propeller twist (PT) values

	Type of	Number of	PT with exo	PT without exo
Material	Pair	base-pairs	atoms in planes	atoms in planes
Nucleosides	All	54	14.7°	14.0°
and	R-R	38	15.7°	15.4°
Nucleotides	Y-Y	16	12.1°	10.5°
Nucleic	All	37	4.4°	4.3°
Acid	Homo	12	1.6°	1.3°
Bases	Hetero	25	5.8°	5.7°

Note - trends within the other classifications are discussed in the text

912 ERRATUM

Results

Further analysis of the results presented previously 1 yielded the results shown in Table 1.

The most noticeable feature of the data, indicated in Table 1, is the very small but systematic reduction of the average propeller twist value in the base-pairs analysed when exocyclic atoms are removed from the base-pair system. This implies that the exocyclic atoms do tend to deviate slightly more than the others from the mean base plane.

The following general trends regarding the effect of removing exocyclic atoms from the calculated base-planes can also be discerned from the data for nucleosides and nucleotides (further to those given in Table 1):

- (i) Y-Y (pyrimidine-pyrimidine) pairs show a greater reduction (12.1° to 10.5°) than R-R (purine-purine) pairs (15.7° to 15.4°);
- (ii) U-U pairs show the largest reduction of all (14.9° to 11.9°);
- (iii) In the Wilson-Tollin (WT) classification², WT(I) [pyrimidine-pyrimidine] reduces most (12.1° to 10.5°, as in (i) above), with WT(VI) ["double-Hoogsteen"] next (15.5° to 14.0°);
- (iv) For the Hobsza-Sandorfy (HS) classes³, the TT(II) (22.8° to 18.0°) and TT(III) (16.9° to 15.0°) groups (comprised mainly of U-U pairs) show the most reduction, with AA(III) [exactly equivalent to WT(VI), see (iii) above, in these data] next.

The overall reduction in propeller twist value for nucleic acid bases is considerably smaller and consequently no notable trends in the reduction of twist in these materials can be discerned.

It is clear from these results that the average propeller twist decreases *more* on exclusion of exocyclic atoms for the least aromatic bases (pyrimidines) than for the more aromatic purines. This is as one would expect, since the additional deviation of exocyclic atoms from the base plane should tend to be more pronounced in the former case. The deviation of exocyclic atoms appears to be on average further out of the plane of the base–*pair*, as opposed to just the plane of the parent base, reflected in the systematic, if small, reduction in propeller twist value obtained when these atoms are excluded from the calculations.

REFERENCES

- 1. Wilson C.C. (1990) Nucleosides and Nucleotides 9, 479-488.
- 2. Wilson C.C. and Tollin P. (1987) Nucleosides and Nucleotides 6, 643-653.
- 3. Hobsza P. and Sandorfy C. (1987) J. Amer. Chem. Soc. 109, 1302-1307.