

Supplementary Information for

## Bicyclic-guanidines, -guanidates and –guanidinium salts: wide ranging applications from a simple family of molecules

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### von Baeyer Nomenclature for Bicyclic Guanidines†

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#### Introduction

A series of bicyclic guanidines reported by Cotton and co-workers were described in two publications<sup>1</sup> according to the von Baeyer convention<sup>2</sup> for naming bridged hydrocarbons and related heterocycles. The rules for the von Baeyer convention of nomenclature are briefly described below for bicyclic derivatives (the rules can also be extended to more complex polycyclic systems). Cotton *et al* made a few minor errors for the locants quoted for their guanidine derivatives. The corrected names together with the relevant compound are also shown below.

#### Naming Hydrocarbon Bicyclic Systems by the von Baeyer Convention

A bicyclic system (which comprises the main ring and main bridge only) is named by:

- the prefix bicyclo- (indicating the number of rings = 2);
- numbers indicating the bridge lengths (*i.e.* number of skeletal atoms excluding the bridgehead atoms) separated by full stops and placed in square brackets. The three numbers are cited in **decreasing order** of size (*e.g.* [3.2.1]);
- the name of the hydrocarbon indicating the total number of skeletal atoms.

#### Numbering of Bicyclic Systems

The atoms of a bicyclic system are numbered from a bridgehead atom *via* the longest path to the second bridgehead atom; numbering of atoms continues round the main ring; and then the main bridge atoms are numbered starting from the lower numbered bridgehead atom (Fig. 1).

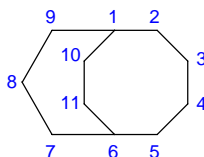


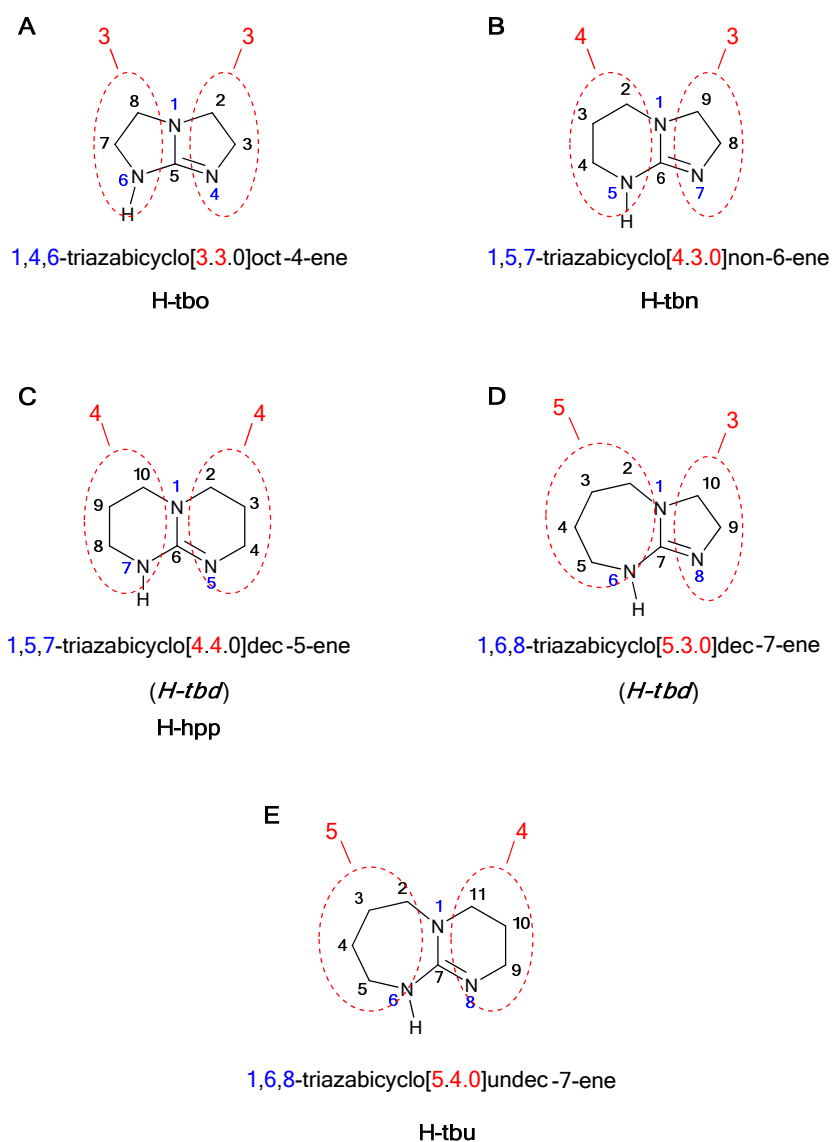
Fig. 1 Bicyclo[4.3.2]undecane

#### Heteroatoms

Low locants are allocated for heteroatoms indicated by replacement terms considered together as a set in **ascending** numerical order. Allocation of locants for heteroatoms, which have replaced carbon atoms, is made after assigning the correct name and numbering for the parent hydrocarbon.

#### Double bonds

Low locants are allocated for double bonds where the atoms of each double bond have consecutive locants. Only the lower of the two locants for each double bond is cited when they differ by one.



**Fig. 2** von Baeyer nomenclature for bicyclic guanidines. Note the abbreviations for the two isomeric compound **C** and **D** are identical as taken from these names. The common abbreviation for 1,5,7-triazabicyclo[4.4.0]dec-5-ene (**C**) is therefore taken from its IUPAC name, 1,3,4,6,7,8-hexahydro-2*H*-pyrimido[1,2-*a*]pyrimidine, H-hpp.

† The International Union of Pure and Applied Chemistry Commission on Nomenclature of Organic Chemistry have published an 'Extension and Revision of the von Baeyer System for Naming Polycyclic Compounds (including Bicyclic Compounds)' with recommendations added in 1999. Full details can be found at the following web-site:

<http://www.chem.qmul.ac.uk/iupac/vonBaeyer/>

#### References

1. F. A. Cotton, C. A. Murillo, X. Wang and C. C. Wilkinson, *Inorg. Chem.*, 2006, **45**, 5493-5500; F. A. Cotton, C. A. Murillo, X. Wang and C. C. Wilkinson, *Dalton Trans.*, 2006, 4623-4631.
2. A. Baeyer, *Ber. Dtsch. Chem. Ges.*, 1900, **33**, 3771-3775; D. R. Eckroth, *J. Org. Chem.*, 1967, **32**, 3362-3365.