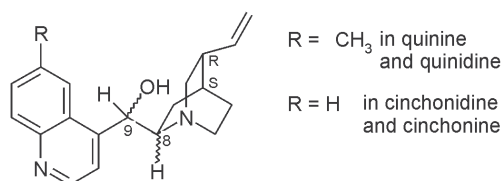


s13.m35.p28 **Cobalt Complexes of Threo-Epipimers of Cinchona Alkaloids: Geometry and Interactions.** I. Tesarowicz, B.J. Oleksyn, *Faculty of Chemistry, Jagiellonian University, Ingardena 3, 30-060 Kraków, Poland. E-mail: ikania@chemia.uj.edu.pl*

**Keywords:** Cinchona alkaloids; Antimalarials; Isomers

The threo-epimers of Cinchona alkaloids, in shortening: epi-alkaloids, are inactive diastereoisomers of the well known antimalarials, erythro-epimers, such as quinine, quinidine, cinchonidine and cinchonine.

In the context of the recently described cobalt complexes of the erythro-isomers [1,2,3] we have obtained the threo analogues in order to compare their geometry and interactions in the crystalline state. The crystal data of three structures determined are shown below.



| Crystal data                        | (epiquininium)-trichlorocobalt(II) ethanolate monohydrate   | (epiquinidinium)-trichlorocobalt(II) monohydrate   | (Epidihydrocinchoninium)-trichlorocobalt(II)                       |
|-------------------------------------|---|--|--|
| Formula                             | C <sub>20</sub> H <sub>25</sub> N <sub>2</sub> O <sub>2</sub> Cl <sub>3</sub> Co · C <sub>2</sub> H <sub>6</sub> O · H <sub>2</sub> O | C <sub>20</sub> H <sub>25</sub> Cl <sub>3</sub> CoN <sub>2</sub> O <sub>2</sub> · H <sub>2</sub> O | C <sub>19</sub> H <sub>25</sub> Cl <sub>3</sub> CoN <sub>2</sub> O |
| System                              | orthorhombic  | monoclinic   | orthorhombic   |
| Space group                         | P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>  | P 2 <sub>1</sub>   | P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>                     |
| a [Å]                               | 12.1180   | 10.1770  | 11.2470  |
| b [Å]                               | 13.5040   | 8.40301  | 13.3070  |
| c [Å]                               | 15.9400   | 4.4040   | 13.6940  |
| β                                   | 90.00°  | 101.1500   | 90.00  |
| V [Å <sup>3</sup> ]                 | 2608.45   | 1208.54  | 2049.50  |
| Z                                   | 4   | 2  | 4  |
| D <sub>x</sub> [g/cm <sup>3</sup> ] | 1.413   | 1.392  | 1.500  |
| μ [mm <sup>-1</sup> ]               | 0.99  | 1.06   | 1.239  |
| λ MoKα                              | 0.71070   |  |  |
| R (F>4σ(F <sub>o</sub> ))           | 0.0403  | 0.0490   | 0.0594   |

In all three complexes the [CoCl<sub>3</sub>] moiety is coordinated with N atom of quinoline. The nitrogen atom of quinuclidine is protonated, which leads to formation of zwitterion. The absolute values of torsion angles of epiquininium and epidihydrocinchoninium are very similar. In epiquinidinium the orientation of the quinoline group in relation to quinuclidine is different than in two other complexes.

The quinuclidine nitrogen atoms and hydroxyl oxygen atoms are proton donors in intermolecular hydrogen bonds with co-crystallizing solvent molecules (epiquinine and epiquinidine complexes) or with chlorine atoms (epidihydrocinchonine).

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s13.m35.p29 **Structure-Property Relationships in Crystal Structures of Molecules with Non-Centrosymmetric Polymorphs.** Graham John Tizzard and Michael Barry Hursthouse, *School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK. E-mail: gjt1@soton.ac.uk*

**Keywords:** Crystal packing; Non-centrosymmetric; Polymorphism

The current interest in the mechanics of crystal structure assembly stems from extensive efforts towards the capability to design or predict crystal structures. This project focuses on the particular feature of non-centrosymmetry in some crystal structures and specifically the assembly of non-centrosymmetric structures by both chiral and achiral molecular systems. To give added focus, a collection of polymorphic 'clusters' has been assembled from the Cambridge Structural Database[1] each of which comprise members of which at least one is a non-centrosymmetric polymorph. The study employs a variety of approaches over and above topology and thus molecular properties such as electrostatic charge distributions and organisation of molecular dipoles have been calculated from *ab initio* computer modelling techniques. In order to facilitate this kind of study, methods are being investigated in which database interrogation and ensuing property calculations can be achieved in an automated manner. Results achieved will be described.

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