s3.m1.p5 **CALCRYS, a new programs in the Tcl/tk based crystallographic package**. L. Urzhumtseva, A. Urzhumtsev, *LCM³B, UPRESA 7036 CNRS, B.P.239, Faculté des Sciences, Université Nancy I, 54506, Vandoeuvre-lès-Nancy, France*.
Keywords: computing crystallography, user-friendly interface, 3D computations.

Crystallographers need a number of simple algebraic calculations in order to obtain lengths, angles, define relations between molecules, transformations of the co-ordinates, etc. These calculations can be done by general means, e.g. either with a usual calculator or with a computer using standard mathematical or big general crystallographic packages. Another possibility is to have a specialised tool, easy to call and to use, fast to address and tuned particularly to these calculations.

A new program in the suite of Tcl/tk based programs (Urzhumtseva & Urzhumtsev, 1996-1999), named CALCRYS, has been developed. This program allows to work with vectors defined either in real or in reciprocal three-dimensional space, expressed either in Cartesian or in crystallographic (fractional) co-ordinates. Unit cell can be defined also either in real or in reciprocal space. When the cell is defined, its parameters in the conjugate space and all metrical tensors are calculated automatically. The optional choice of the orthogonalisation agreement allows to establish automatically the orthogonalisation and deorthogonalisation matrices. This crystallographic information is presented permanently at the screen.

The available algebraic operations include the calculation of a linear combination of vectors, their scalar and vector product (taking into account the corresponding metrical tensors), the product of a matrix by a vector or by another matrix, a linear combination of matrices, matrix inversion, matrix determinant etc. These operations are gathered in a menu displayed near the set of work windows containing the data with which these operations are executed. One more field contains a number of "memory cell" which allow to save intermediate results (any mixture of numbers, vectors or matrices) and to use them later. An information can be inserted into the working windows in several ways : copied from the crystallographic field, from the memory cells, directly typed or read from a file.

The program CALCRYS is written in Tcl/Tk (Osterhaut, 1993). It can be ran under UNIX on an SGI computer, on a DEC Alpha station, or on an IBM PC under Windows, with the Tcl/Tk libraries installed. The program can be also run on Macintosh with a X-terminal emulator, e.g. *exodus*[1].

[1] Ousterhout J.K. "Tcl and the Tk Toolkit". (1993) Addison-Wesley Publishing Company.

s3.m1.p6 ***Ab initio* DFT Calculations on NAD^+ and $NADP^+$.** N. Muzet, B. Guillot, C. Jelsch & C. Lecomte *LCM³B-CNRS-UHP Vandoeuvre-les-Nancy FRANCE.* E. Artacho *Instituto de Ciencia de Materiales Nicolàs Cabrera and Departemento de Fisica de Materia Condensada, Madrid, SPAIN.*
Keywords: deformation density maps, DFT, NAD^+ and $NADP^+$.

Ab initio crystal and single molecule calculations for NAD^+ and $NADP^+$ have been performed at DFT level using the Siesta package [1].
The molecular structure of NAD^+ is taken from the very-high resolution X-ray diffraction data of NAD^+ triclinic crystal [2]. Crystal water molecules are included in the calculation.

For $NADP^+$, the molecular structure has been extracted from the Aldose Reductase high-resolution X-ray diffraction data [3]. Hydrogen atoms have been added to the water oxygens from the crystal and positions have been optimized by molecular dynamic simulation at 100 K, using AMBER software.

For all molecules, Siesta standard double zeta basis sets with polarization have been used, and periodic calculations have been performed for the NAD^+, using the crystal triclinic parameters.

Deformation density maps of both molecules have been calculated in order to compare with experimental results and to assess the use of fragments transferability [4].

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[2] B. Guillot, C. Jelsch & C. Lecomte, (2000), *Acta Cryst.*, C56, 726-728.
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[4] Jelsch C., Teeter M.M., Lamzin V., Pichon-Pesme V., Blessing R.H. & Lecomte C., (2000), Proc. Nat. Acad. Sci. USA. 97, 3171-3176.