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Introduction to JANA2006

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JANA2006 is a new version of crystallographic compu-ting system JANA [1] originally developed for incom-mensurately modulated structures. During more than 20 years of development it became widely used unified system for structure analysis of periodic and aperiodic crystals with emphasis on solving difficult structures. This unifying trend is followed further in JANA2006.

The main improvement of the new system consists in complete generalization of multiphase and multisource crystallographic data input. Thus the new system can combine for instance X-ray single crystal data with neutron powder data even for samples containing several phases in different ratios. An example utilizing combination of data will be given in the presentation. The Rietveld refinement option as already implemented into JANA2000 offers the standard profile functions and anisotropic tensors for strain profile broadening. Fundamental approach to profile fitting [2] is an important new feature in JANA2006 giving more exact physical sense to profile parameters and connecting them better with the real experimental arrangement. Support for TOF data was added, too. JANA2006 will support refinement of magnetic structures. The superspace approach to handle mutually magnetic and structural modulations is under development. Charge flipping generalized for superspace [3] will be integral part of the program as an alternative solution method especially useful for modulated structures. New graphical interface attempts bringing multilevel menu-driven control to more intuitive one level interface. Dynamical elements were added like updating of Fourier contour plots or powder profiles during refinement. The automatic tasks like (super)space group determination and graphical way of adding hydrogen atoms were improved. Work with simple structure is also better supported, especially creation of CIF output conforming better to current requirements of Acta Crystallographica E,C. From the technical point of view JANA2006 differs significantly of the previous versions by possibility to allocate memory dynamically (it uses FORTRAN95) and by using precompiled binaries for LINUX and MAC OS X operating systems. All JANA programs are freeware. JANA2006 is currently available in beta version by request; the first publicly available beta version is expected at the end of this year.

[1] http://www-xray.fzu.cz/jana/
[2] Cheary,R.,W. & Coelho,A.,A.(1998). *J.Appl.Cryst.,* 31, 851-861
[3] Palatinus,L. (2004). *Acta Cryst.* A60, 604-610.

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Superspace embedding of sheelite-like structures

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The superspace concept is applied with the aim to describe and extend the sheelite-like structure family with a single (3+1)D model. Two sheelite-like incommensurately modulated $A'A''[MoO_4]_2$ structures have been solved and refined in the monoclinic distorted sheelite-like unit cell and superspace group $I2/b(\alpha\beta0)00$. $KNd[MoO_4]_2$: a = 5.5202(2) Å, b = 5.33376(5) Å, c = 11.8977(3) Å, γ = 90.9591 (7)°; **q** = 0.57789(4)**a*** - 0.14748(6)**b***. $KSm[MoO_4]_2$: a = 5.5300(2) Å, b = 5.33005(5) Å, c = 11.7873(3) Å, γ = 91.1401 (7)°; **q** = 0.56688(4)**a*** - 0.1392(6)**b***). These structures are described as a distorted cubic face centred (*fcc*) double cell with the lattice parameter $a \approx 5.5 \pm 0.2$ Å for one *fcc* cell. Both A and MoO_4 building units are located at the junctions of the double *fcc* cell. Two independent variables have been selected in order to characterise the structural individualities: the occupation of the A-cation and the modulation vector $\mathbf{q} = \mathbf{a}^* + \mathbf{b}^*$. The first one defines an ordered distribution of cations in the A-position. The second one defines the composition modulation wave between $\{A'[MoO_4]\}$ and $\{A''[MoO_4]\}$. This is also reinforced from published data on the incommensurately modulated structure $Ag_{1/4}Pr_{5/4}(MoO_4)_2$ [1]. According to our definition, the general sheelite-like superstructure type is attributed the following conditions: (1) The double *fcc* (average) cell with the lattice parameters $a \approx b \approx 5.5 \pm 0.5$ Å, $c \approx 2a$, γ is close to 90° belongs to the superspace group $I2/b(\alpha\beta0)00$. (2) The average structure is defined by the atomic coordinates of sheelite ($CaWO_4$) for the compounds with general formula $(A',A'')_{n-\Delta A}[(X',X'')O_4]_{n-\Delta X}$, where $\Delta A \geq 0$ and $\Delta X \geq 0$ define possible vacancies in the corresponding positions. The commensurate and incommensurate structures of the family are determined by the variation of the **q**-vector and the occupation functions of A and XO_4 building units. The displacement modulations of the atoms depend on the chemical composition of the compounds. About 10 different known commensurate structures with A = K, Na, Bi, Zr, Y, Ln and X = Mo, W, V, Fe can be attributed to the sheelite-like superstructure type. Several compounds can be found in the JCPDS database, but without indexation, which can be interpreted with our superspace model. As an example, we refined the unit cell parameters and the **q** vector and finally indexed the powder diffraction pattern of $KEu(MoO_4)_2$ (JCPDS PDF2 # 31-1006).

[1] V. Morozov *et al*. *J. of Solid State Chemistry* 179 (2006) 1172-1180.