s2.m1.p7 **Investigation of low-temperature superstructure and electron density of a'-NaV_2O_5.** S. Geupel, J. Luedecke and S. van Smaalen, *Laboratory of Crystallography*, *University of Bayreuth*, *D-95440 Bayreuth*, *Germany*.
Keywords: low-dimensional compound, maximum-entropy-method, electron density.

a'-NaV_2O_5 has attracted much attention as a low-dimen-sional compound exhibiting a phase transition from a paramagnetic state towards a magnetically ordered state below T_c = 34 K, as shown by susceptibility measurements [1]. The magnetic ground state is connected with a commensurate lattice distortion leading to a F-centered ($2a \times 2b \times 4c$)-supercell (space group *Fmm*2). It contains three symmetry-independent V atoms arranged in modu-lated ladders with zigzag charge order V^{4+}/V^{5+} and non-modulated ladders with mixed valence state $V^{4.5+}$ [2,3], whereas the centrosymmetric room-temperature phase (space group *Pmmn*) is characterized as a mixed-valent insulator with only one symmetry-independent $V^{4.5+}$ site. Consequently, the phase transition in a'-NaV_2O_5 cannot be regarded as a simple spin-Peierls transition, but must be accompanied with a charge ordering which localizes the V 3*d*-electrons on one site of each rung of the lad-ders. One possible explanation for the observed magne-tic ordering is the formation of spin-singlet clusters, in-volving two V^{4+} atoms on next-nearest-neighbour lad-ders and four $V^{4.5+}$ atoms on the non-modulated ladder in between [4].

We report about new structure refinements of the low-temperature phase using a combination of three single-crystal data sets measured within different 2θ ranges. It is shown that the refinement of the superstructure is successfully only within the so-called superspace approach, but it is unstable for the conventional supercell descrip-tion because most of the measured second-order satellite reflections are of zero intensity. Furthermore, we have now estimated more accurate values for the valencies of V atoms by means of the the bond-valence method. Our results point out that the charge order is probably incomplete, and includes V^{4+d} and V^{5-d} atoms with $d \approx 0.14$ [5].

Finally, we present first results of electron density studies of the low-temperature phase using the Maximum-Entropy-Method and discuss them in relation to the proposed charge ordering.

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s2.m1.p8 **Preliminary Results for a Charge Density Study of Estrone.** D. Parrish, N. Wu, E. Zhurova, and A.A. Pinkerton. *Department of Chemistry, University of Toledo.*
Keywords: estrogen charge density.

A charge density study has been carried out on estrone, a member of the estrogen hormone family. The estrogens have been strongly linked to the initiation and progress of breast cancer. The mechanism by which these hormones influence gene expression is unknown. It has been postulated that the differences in electrostatic potential of the estrogen derivatives elicit the diverse responses seen. It is anticipated that comparative charge density studies of the different derivatives, the first of which is presented here, will yield information about what electronic features could be responsible for certain characteristic activities.

The data was collected on a Bruker platform detector equipped with a 2K area detector using AgKα radiation. The temperature of the crystal during the measurement was 92K. Data was collected at a distance of 6.00 cm, which required two detector positions of 2θ = –20° and -65° resulting in >90% coverage out to sin θ/λ=1.33 A. Omega scans of 0.2° were carried out at several different phi settings. Data integration was performed with SAINT 7 and an absorption correction was applied using SADABS. Statistical analysis was performed with SORTAV. The multipole refinement was done using the XD software package. The final refinement yielded $R_{obs}(F^2)$= 0.03, $R_{all}(F^2)$=0.07. Representative maps of the deformation density will be presented.