**UM518 (UM450 Update!)**

**Experimental:**

A black plate with approximate dimensions 0.145 x 0.127 x 0.044mm³ was placed and optically centered on the Bruker SMART1000 single crystal CCD-diffractometer. The crystals' initial unit cell parameters and crystal orientation matrix were determined from a least-squares analysis of a random set of reflections collected via three sets (30 frames/set) of 0.3° wide ω-scans that were well distributed in reciprocal space. The intensity data were collected with 0.3° wide ω-scans (40sec/frame) and a crystal to detector distance of 4.97cm thus providing a complete sphere of data to 55° in 2θ. The unit cell was now optimized using all of the frames from the initial series (606 frames) and a random set of frames chosen from the subsequent data collection runs and used throughout the data reduction sequence. A total of 8442 data (±h±k±l) were corrected for Lorentz and polarization effects using the SAINT+¹ data reduction program with 1188 unique [R(int)=0.0591]. An empirical absorption correction was applied to the data based upon equivalent reflection measurements using Blessing’s method in the program SADABS².

XPREP³ now checked the cell symmetry, confirmed the systematic absences that clearly indicated the centro symmetric rhombohedral space group R-3 (no. 148) and set up the initial files. The structure was determined by direct methods with the successful location of the Sr and V atoms using the program XS⁴. The structure was refined with XL⁵. The remaining atoms were located from two subsequent difference-Fourier maps. After several cycles of refinement, all of the atoms were refined anisotropically. The final structure was refined to convergence [Δ/σ ≤ 0.001] with R(F)=4.37%, wR(F²)=11.18% and GOF=1.099 for all 1188 unique reflections [R(F)=4.08%, wR(F²)=11.05% for those 1080 data with Fo > 4σ(Fo)]. A final difference-Fourier map possessed several peaks that appear to be ‘ghosts’ and are as large as |Δρ| ≤ 3.23eÅ⁻³, indicating that the structure is both correct and complete.

The function minimized during the full-matrix least-squares refinement was \( \Sigma w(Fo^2-Fc^2) \) where \( w=1/[σ^2(Fo^2)+(0.1220*P)^2] \) and \( P=(max(Fo^2,0)+2*Fc^2)/3 \). An empirical correction for extinction was attempted but found to be negative and not applied.

**References:**

1. Saint+ Data Reduction program. Bruker Analytical X-ray Systems, Madison, Wisconsin, USA.
Table 1. Crystal data and structure refinement for Sr6V9S22O2.

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<td>R indices (all data)</td>
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<td>Largest diff. peak and hole</td>
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Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2$ $\times 10^3$) for Sr6V9S22O2. U(eq) is defined as one third of the trace of the orthogonalized U tensor.

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Table 3. Bond lengths [Å] and angles [°] for Sr6V9S22O2.

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Sr(1)#13-O(1)-Sr(1)#1
Sr(1)#4-O(1)-Sr(1)#1

Symmetry transformations used to generate equivalent atoms:

#1 -x+5/3,-y+1/3,-z+1/3  #2 -x+y+1,-x+1,z  #3 -y+2,x-y,z
#4 x-y+2/3,x-2/3,-z+1/3  #5 -y+1,x+y,z  #6 x-y,x-1,-z
#7 -x+2,-y+1,-z  #8 -x+2,-y,-z  #9 -x+y+2,-x+1,z
#10 -y+1,x-y-1,z  #11 y+1,-x+y+1,-z  #12 x,y-1,z
#13 y+2/3,-x+y+1/3,-z+1/3  #14 x,y+1,z  #15 -x+y+2,-x+2,z
#16 y+2/3,-x+y+4/3,-z+1/3  #17 -x+8/3,-y+4/3,-z+1/3

S10
Table 4. Anisotropic displacement parameters (Å² x 10³) for Sr6V9S22O2. The anisotropic displacement factor exponent takes the form: \(-2\pi²[ h^2 a^*^2 U^{11} + ... + 2hk a^* b^* U^{12} ]\)

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