

Breaking Boundaries: Novel Tridecavanadate Polyoxometalate with a Unique Sixfold Tetradentate Coordination Capacity for Lanthanum(III) and a Twofold Bidentate Decavanadate Ligand in a Single Compound

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Supporting Information

Fig S1. FT-IR spectrum of **1a**

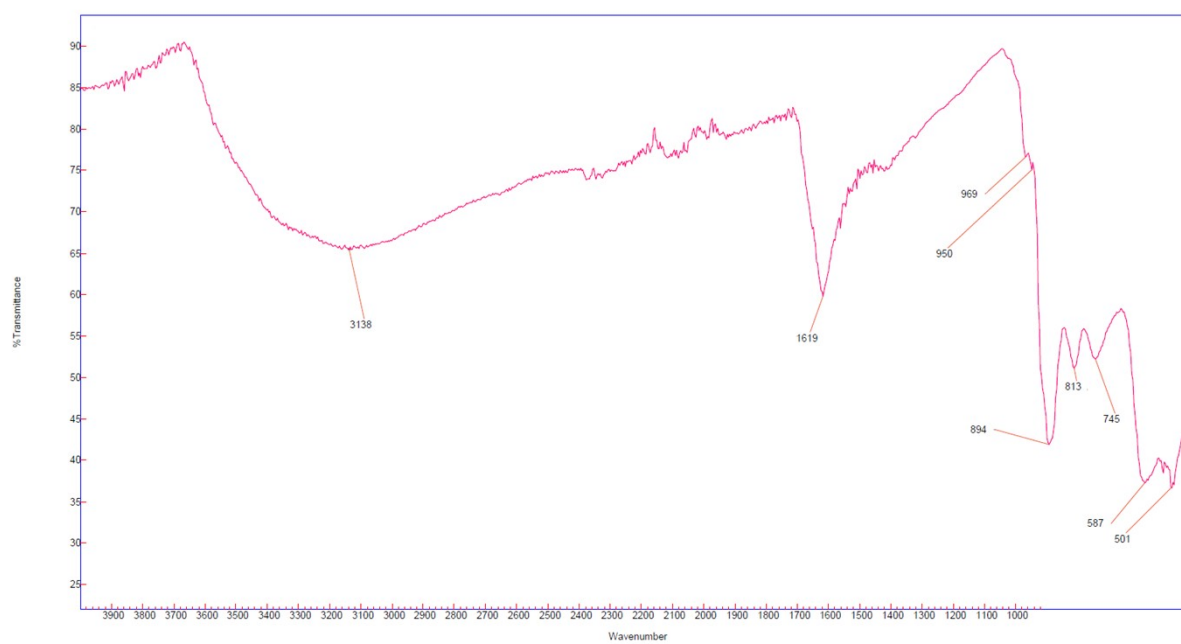
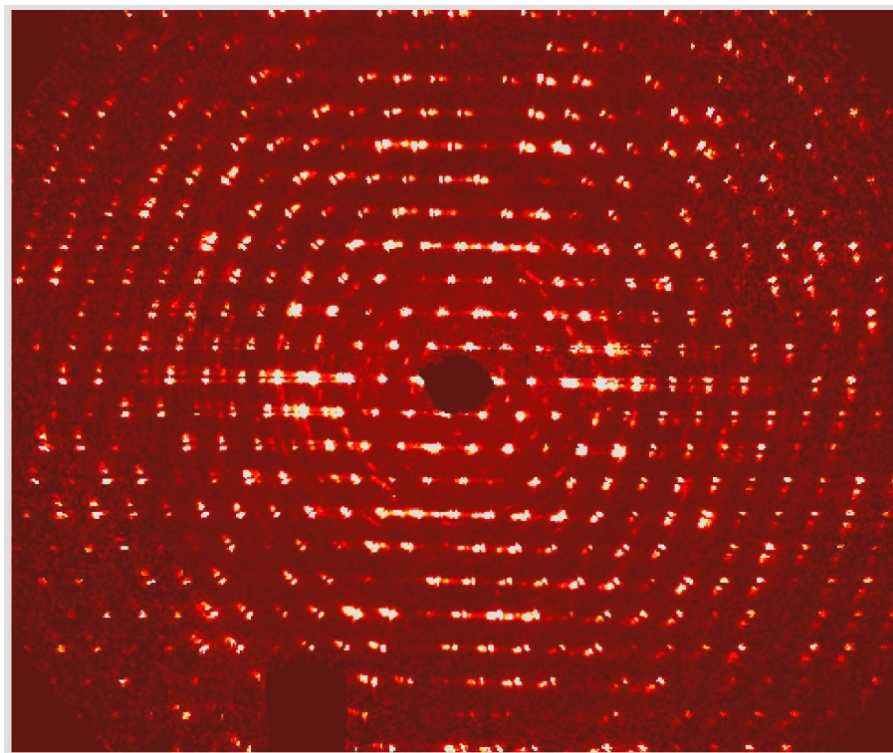


Fig S2. Comments to the crystal structure of **2**

The compound crystallizes as a split (twinned) crystal and the quality of the crystal was not quite good, which can be observed from the reciprocal lattice layer constructions, showing twinned spots:



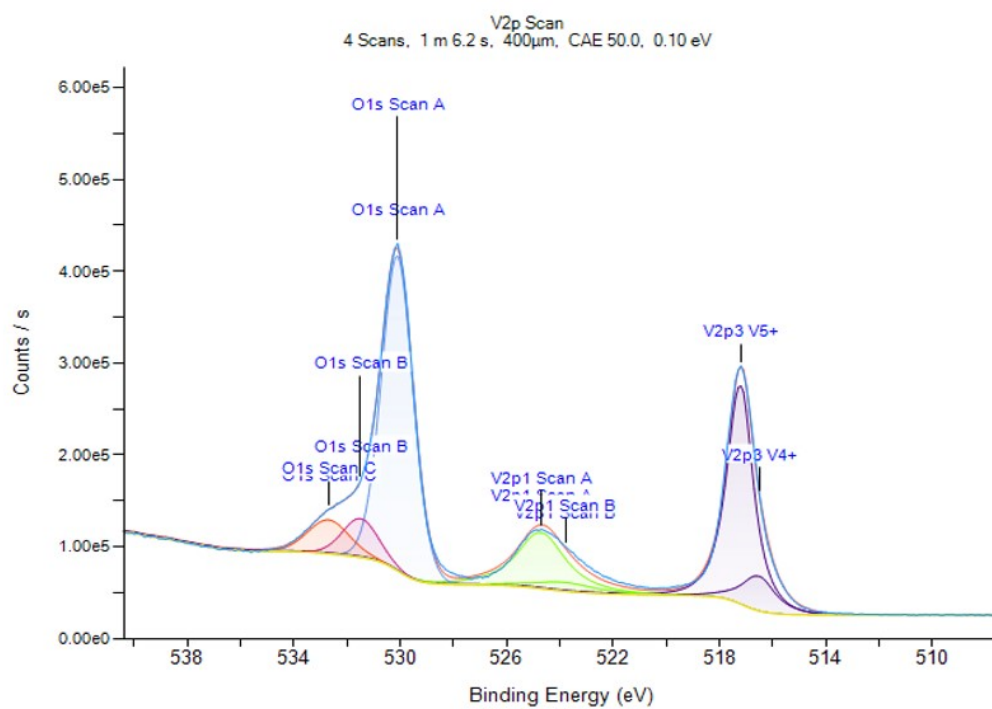
Twin integration was performed to the data set.

Twin integration results:

1. The data set was treated for the twin behavior of the crystals.
2. The calculations suggest a 1.75-degree rotation of the lattice to get the second twin component.
3. Twin treatment revealed that the crystals might be split crystals while it is technically not a twin, in a real sense.
4. The residual electron density near La could be a consequence of the effects of twinning.

The second product **2** is a rough structure and do not get into many details about the geometry, bond lengths, etc; and this incomplete structure is added just to prove the product. Yet due to its uniqueness regarding the coordination mode of decavanadate we found appropriate to publish at least the connectivity of the atoms.

Fig. S3 XPS scan of sample **1a**



Full measurement details in a separate file.