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Keywords: chirality, chiral, borate

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Recent developments in the SuperNova dual source micro-focus diffractometer.

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The introduction of the **SuperNova** in late 2008 being the first dual wavelength micro-focus diffractometer gave a tremendous boost to the capabilities and throughput for in-house crystallographic research. The combination of the high intensity Cu and Mo micro-focus sources (50W) co-mounted along with a 135mm Atlas CCD detector allows for true flexibility on a per-experiment basis.

Continued research and development in core technologies used in the **SuperNova** means that key aspects of the instrument have been updated and improved since its initial launch. Here we would like to highlight the overall benefits of these evolutionary changes and refinements in both hardware and software by presenting a number of absolute configuration determination studies. The examples presented include a broad spectrum of materials with greatly varying anomalous signal, including the first, purely hydrocarbon based molecule's experimental chirality determination using Bayesian methods.

Keywords: absolute configuration determination

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A three-dimensional framework structure of vanadium and 1,2,4,5-benzenetetracarboxylate

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Blue block crystals were obtained from the hydrothermal synthesis in aqueous solution of vanadium pentoxide, titanium tetraisopropoxide and 1,2,4,5-benzenetetracarboxylic acid in the molar ratio 1:2:2 at 150°C for 4 days, and structurally analyzed by single crystal X-ray diffraction. The interest in solving this structure is the difficulty in defining the correct space group. The unit cell parameters are consistent with a tetragonal unit cell, yet the systematic absence data cannot unambiguously identify an appropriate space group.

Assuming the structure to be orthorhombic with *a* and *b* approximately equivalent provides for the space group $P2_12_12_1$ with $a = 11.1302(6)$, $b = 11.1307(6)$, $c = 13.4114(7)$ Å, $Z = 4$ and $V = 1660.457(15)$ Å³. To solve the structure, both racemic and pseudo merohedral twin law were applied; the Flack parameter for the current refinement is 0.20(8), which indicates inversion twinning. However, the best model obtained so far refines to give $R_1 = 0.1286$, and further investigation is needed. The structure contains two crystallographically-independent vanadium atoms in octahedral geometry coordinated by four carboxylate-oxygen atoms from fully deprotonated 1,2,4,5-benzenecarboxylate ligands in the equatorial positions and two aqua ligands occupying the axial positions generate the three dimensional framework structure.

Keywords: pseudo merohedral twin, vanadium carboxylate, framework structure

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Synthesis and structural characterization of two new isoindol derivatives

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Isoindol derivatives are versatile intermediates for the synthesis of a variety of bioactive compounds, and possess a broad spectrum of biological activity such as insecticidal, antibacterial, antibiotic, antitumor, antifungal, psychotherapeutic, antihypertensive, HIV and other activities. In this study, two new derivatives of Isoindol, N-(1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2H-4,7-methanoisoindol-2-yl)-2,2-dimethylpropanamide and 4,8-Methano-3-(2,5-dimethoxyphenyl)-6-(methylamino)4,4a,8,exo-8a-tetrahydro-exo-3aH isoxazolo [5,4-f]isoindole-5,7(6H,7aH)-endo-dione, have been synthesized and characterized by elemental analysis, FT-IR, UV-Vis and 1H NMR spectroscopy. The crystal structure of this compounds has been determined by single crystal diffraction method. The first compound (C₁₄H₁₈N₂O₃), which is an oxalamide derivative, crystallized in the orthorhombic system with space group Pca21, $a = 24.038$ (2) Å, $b = 9.3387$ (7) Å, $c = 12.3004$ (9) Å, $Z = 8$. The final R value is 0.0066 for 5227 measured reflections. The compound has two molecules in the asymmetric unit, is a chiral compound with 8 stereogenic center. This compound occurs non-centrosymmetric dimeric structure with N-H...O type H-bond. The crystal structure of the compound is stabilized by intermolecular N – H...O type and intramolecular N – H...O, C – H...O type H-bonds, also C – O...pi weak interactions[1,2]. The second compound (C₁₉H₂₀N₂O₅) is an isoxazoline derivative, crystallized in the monoclinic system with space group P21/n, $a = 9.7183$ (1)Å, $b = 13.1735$ (2) Å, $c = 13.2880$ (2)Å, $\beta = 94.058$ (1)°, $Z = 4$. The final R value is 0.0036 for 3404 reflections. The molecule adopts Z-configuration. The structure is a chiral compound with 4 stereogenic center. Molecule occurs the fusion of the isoxazoline ring and dicarboximide onto norbornane unit. The crystal structure is stabilized by C – H...O type intra-molecular, C – H...N and C – H...O type inter-molecular interactions. In the crystal structure intermolecular N – H...N and C – H...O hydrogen bonds link the molecules to form an infinite one dimensional polymeric chain along b-axis. Crystallographic results are consistent with the literature [3], [4].