

structure and characterization, polycrystalline X-Ray diffraction

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#### Structural and thermal analytical study on *trans*-diammine-bis(nitrito) complex of Pd(II) and Pt(II)

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Aqueous ammonia solutions of Pd(NH<sub>3</sub>)<sub>2</sub>(NO<sub>2</sub>)<sub>2</sub> and Pt(NH<sub>3</sub>)<sub>2</sub>(NO<sub>2</sub>)<sub>2</sub> are used, after impregnations and heat treatments between 150 and 350 °C, for a successful sensitization of SnO<sub>2</sub> layers for CO gas [1]. In order to identify the active sensing chemical species of residues from the Pd or Pt solutions, a detailed study on thermal decomposition of solid *trans*-Pd(NH<sub>3</sub>)<sub>2</sub>(NO<sub>2</sub>)<sub>2</sub> (**1**) and *trans*-Pt(NH<sub>3</sub>)<sub>2</sub>(NO<sub>2</sub>)<sub>2</sub> (**2**), crystallized from the used solutions, has been carried out. Compounds **1** and **2** have been characterized by their FTIR spectra and XRD profiles. Their composition and *trans* configuration have also been identified by reference IR spectra [2] and XRD reference patterns (PDF 00-45-598 and PDF 00-54-155) [3]. The crystal and molecular structure of *trans*-Pd(NH<sub>3</sub>)<sub>2</sub>(NO<sub>2</sub>)<sub>2</sub> (**1**) has been determined by single crystal X-ray diffraction (R = 0.0515). The obtained crystallographic data of the triclinic crystals of (space group *P*-1, *a* = 5,003(1) Å, *b* = 5,419(1) Å, *c* = 6,317(1) Å, α = 91.34(2)°, β = 111.890(10)°, γ = 100.380(10)°) has been found close to that was reported earlier [4]. A better understanding of mechanism and dynamics of the gas evolution from these solid complexes **1** and **2** probably sensitive to shock seems to be essential during a scaling up of sensor fabrication.

#### References

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#### Crystal structure of synthetic hydrotungstite, WO<sub>2</sub>(OH)<sub>2</sub>(H<sub>2</sub>O)

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Hydrotungstite, WO<sub>2</sub>(OH)<sub>2</sub>(H<sub>2</sub>O) or H<sub>2</sub>WO<sub>4</sub>(H<sub>2</sub>O) (PDF 00-016-0166 and 00-018-1420) occurs as an alteration product in the oxidized zone of a hydrothermal tungsten ore deposit at the Calacalani mine in Bolivia, and thin films of hydrotungstite have been used as humidity sensors. It is reported to crystallize in *P2/m* with *a* = 7.379(5), *b* =

6.901(5), *c* = 3.748(5) Å, and β = 90.36(16)°. The powder pattern of a greenish yellow precipitate from an inductively-coupled plasma (ICP) specimen preparation of a W-containing sample matched that of hydrotungstite well, but the unit cell and powder pattern were more complicated than had been reported. Application of lattice matching techniques to the reported unit cell yielded the chemically-plausible analogue “yellow molybdic acid”, MoO<sub>3</sub>(H<sub>2</sub>O)<sub>2</sub>, which has the ICSD formula type AX5. A further search for Mo-containing compounds having this formula type yielded the mineral sidwellite, MoO<sub>3</sub>(H<sub>2</sub>O)<sub>2</sub>, which crystallizes in *P2<sub>1</sub>/n* with *a* = 10.487(1), *b* = 13.850(1), *c* = 10.617(1) Å, and β = 91.62(9)°, and has been studied using neutron powder diffraction. The sidwellite cell is an 8 × supercell of the reported hydrotungstite cell, and the sidwellite structure served as a good initial model for a Rietveld refinement of the hydrotungstite structure. The hydrogen positions were determined by a quantum chemical geometry optimization, which permitted analysis of the hydrogen bonding pattern. The structure consists of corner-sharing layers of tilted WO<sub>6</sub> octahedra in the *ac* plane. Pointing into the interlayer region *trans* to each tungsten atom are a coordinated water molecule and a W=O group. The interlayer region is occupied by water molecules, which are hydrogen bonded to the layers. Hydrotungstite is properly formulated [WO<sub>3</sub>(H<sub>2</sub>O)](H<sub>2</sub>O). The structure of the mineral tungstite, WO<sub>3</sub>(H<sub>2</sub>O), has been reported, but the topologies of the layers in sidwellite and tungstite differ. A combination of quantum calculations and Rietveld refinement was used to determine the best model for the topology of the hydrotungstite layer. The quantum calculations help establish the relative energies of hydrotungstite and tungstite.

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#### Periodic properties of atomic matter

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A relationship between the periodicity of atomic matter with natural-number patterns was unveiled recently<sup>1</sup>. Almost a century ago W.D. Harkins<sup>2</sup> noted that for stable nuclides the proton/neutron ratio converged to a value *Z/N* of 0.62 (the neutron had not been discovered at that time). This value has now been recognized as the number tau, well known in number theory and popularly referred to as the ‘golden ratio’<sup>3</sup>. The periodic nature of the stable nuclides has also been demonstrated in other ways, such as by considering experimentally observed properties of nuclides including the nuclear binding energy (NBE), spin, abundance and thermal cross section. There is an undeniable link to number theory: Fibonacci numbers, the golden ratio and Farey sequences, established without any assumptions about the nuclear properties of the 264 known stable nuclides. Fig. 1. *A/N* or *A/Z* vs. mass number for nuclides with *A*=4*n* converge to limiting values close to tau+2 or tau+1.

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