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Application of statistical methods for the prediction of properties of organic solid forms

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We are investigating the application of appropriate statistical methods for the prediction of the formation and properties of organic solid forms, taking advantage of the possibility to determine structures and properties of family sets of organic solid forms using High Throughput Chemical Crystallography. Statistical models are being built to relate quantitative descriptors of molecular or crystalline structure to the classification of compounds, and to predict measured properties of the compounds, such as melting point and enthalpy of fusion. In many of these studies, a large number of quantitative variables are available as potential predictors of a response. The sizes of available datasets and feasible experiments (small to medium), often result in there being more potential descriptors than data points. We are therefore exploring the selection of statistically relevant subsets of the possible descriptors. A further complication is the need to consider nonlinearities in the statistical models and interactions between the variables. A variety of data forms are being considered, including binary data for the classification problem, categorical data when considering the occurrence of polymorphs and continuous data for measured properties. Appropriate statistical methods are being developed, where necessary, and applied to each situation, based on methods such as generalised linear and additive models, recursive partitioning and classification trees, and ensemble models. The performance of different methods are being critically assessed and compared. The poster will present results obtained so far.

Keywords: statistical methods, crystal structures, property prediction

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High hardness and incompressibility in transition metal borides

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Transition metal borides have recently gained high interest as potential superhard materials. Despite the high costs for the transition metals, their synthesis is comparably facile and can be done at ambient pressure conditions, what favours them for example against c-BN or advanced nanocomposite materials for a potential use in industrial applications. In a systematic study, we synthesized borides of Ru, W, Re, and Os. The crystal structures of these materials are characterized by a different packing of transition metal and flat and/or puckered boron layers. The mechanical properties were determined by microindentation as well as compressibility measurements using diamond-anvil cells and synchrotron radiation. The observed

properties of the materials can be understood based on their crystal structures and the chemical bonding. The analysis of the chemical bonding of these compounds by means of the electron localization function (ELF) revealed a high degree of covalent boron-boron bonding as a necessity for a high hardness. On the other hand, as it is well known, a high electron concentration yields to an incompressible material. Therefore, OsB was found to be the most incompressible, WB₄ the hardest of the investigated materials. A good compromise between incompressibility and hardness was found for WB₂, (W,Os)B₂ and the isoelectronic ReB₂. We thank the staff of the MS beamline at Swiss Light Source (SLS at PSI, Villigen, Switzerland) for experimental assistance

Keywords: borides, bulk modulus, microhardness

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Structure and magnetic study of solvated and non-solvated spin crossover complex [Fe(SalEen)₂]ClO₄

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The water solvated [Fe^{III}(SalEen)₂]ClO₄·0.5H₂O (**1**) and non-solvated [Fe^{III}(SalEen)₂]ClO₄ (**2**) complexes were synthesized and structure characterized (SalEen = N-(2-ethylamino)ethyl-salicylaldehyde). Complex **1** crystallizes in the polar orthorhombic space group *Fdd2* with cell parameters $a = 18.4301(7)$, $b = 55.7300(20)$, $c = 9.9021(3)$ Å, $V = 10171.1(6)$ Å³, $Z = 16$, while complex **2** crystallizes in the monoclinic space group *P2₁/c* with $a = 9.9440(2)$, $b = 21.1875(5)$, $c = 12.3637(3)$ Å, $\beta = 104.311(1)^\circ$, $V = 2524.1(1)$ Å³, and $Z = 4$. The water molecule induces a very different molecular packing situation which causes distinct magnetic property between the solvated and non-solvated complexes. The thermal dependent magnetic measurement shows gradual spin transition property for both complexes, both are in the high spin (HS) state $S = 5/2$ at 350 K and convert to the full low spin (LS) state $S = 1/2$ below 30 K for **1** ($T_{1/2} = 155$ K) and 120 K for **2** ($T_{1/2} = 230$ K). A two-step spin transition is interested found in complex **1**, which represents the first Fe(III) system with such behavior. Crystal structures of the LS state at 25 K for **1** and at 100 K for **2** are collected for comparison to the HS state structures at 300 K. The bond lengths associated with the FeN₄O₂ octahedron in the HS and LS states are consisted with the magnetic result. The Fe-N_{avg} and Fe-O_{avg} differences are 0.148 and 0.034 Å shorter for **1** and 0.132 and 0.027 Å shorter for **2** in the LS state, respectively. Also the octahedral distortion parameters Σ and Θ , defined as the sum of the absolute values of the deviation from 90° of the 12 cis angles and deviations from 60° of the 24 possible angles in the coordination sphere, show the more closely to normal octahedral environment in the LS state as expected.

Keywords: structural and magnetic phase transitions, magnetic behaviour, single-crystal characterization

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Structural-microstructural & magnetic properties relationships of In_{1.0}Fe_{0.1}Te_{0.9}, In_{1.0}Co_{0.1}Te_{0.9}

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