loss/reduction of its haemolytic, phospholipase C and sphingomyelinase activity.

Keywords: bacterial toxins, crystal structures, site-directed mutant

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An Improved Method for Calculating Ligand Solid Angles

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A new approach has been developed to numerically calculate solid angles of the ligands in organometallic complexes. The novelty of the method is in using atomic radii corresponding to the distance where the Morse potential becomes zero, rather than in using the "typical" atomic van der Waals radii corresponding to the minimum of the Morse function. The calculated values include the ligand solid angles, the corresponding cone angles (rather than Tolman cone angles), the ligand special overlaps, ligand overshadowing, and the molecular solid angle. In addition, the calculated solid and cone angles are normalized to a Metal-Ligand distance of 2.28 Å to allow facile comparison of ligand steric demands in complexes of different metals with different compositions of coordination spheres. The new approach has been implemented in the program Solid-G and solid angles parameters with standard deviations have been computed for most common ligands such as cyclopentadienyl and tri-substituted phosphines. The new approach allos to evaluate the conformational flexibility of the ligands.

Keywords: solid angle, **organometallic complexes**, **ligands**

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The Perpendicular Magnetic Anisotropy Effect and the Directional Structure Ordering of $CrPt_3$ the Epitaxial Films

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The epitaxial cubic symmetric $CrPt_3$ films exhibit a perpendicular magnetic anisotropy (PMA) with large Kerr rotation angles. In order to understand the PMA effect of such a cubic $CrPt_3$ thin film, the directional chemical order parameters S and polarization dependent x-ray absorption fine spectroscopy (XAFS) were measured in both in-plan and plane-normal directions. The best PMA effect can be found when the plane normal order parameter is largest while the in-plane one is still low. At the same time, Cr-Cr bond-distance have slight distortion by XAFS analysis. This anisotropic directional long range chemical order might be due to the anisotropic interdiffusion and the compound formation between the Cr and Pt layer. For a short-range order analysis, the PMA effect might be attributed to the difference of the Cr-Cr bond-distance between plane-normal and in-plane directions.

Keywords: ordering, magnetic properties, CrPt alloy

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Distribution of Sr Ions in Tungstenbronze-type-like $(Ba_{1-\alpha}Sr_\alpha)_{6-3x}R_{8+2x}Ti_{18}O_{54}$ (R = Sm, Nd) Solid Solutions

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Tungstenbronze-type-like $(Ba_{1-\alpha}Sr_\alpha)_{6-3x}R_{8+2x}Ti_{18}O_{54}$ (R = rare earth) solid solution is one of the microwave dielectric materials. The crystal data is as follows: orthorhombic, *Pbnm* (No. 62), $a \approx 12$, $b \approx 22$, $c \approx 7$ Å and $Z = 2$. The crystal structure of the solid solution is composed of two kinds of large cation sites: four pentagonal sites with Ba ions and ten rhombic sites with Ba, Sr and R ions in the framework formed by TiO_6 octahedron.

These single crystals for R = Sm and Nd system were synthesized by conventional cooling method and FZ method, respectively. The X-ray diffraction data were obtained by a diffractomater with imaging plate (Rigaku; R-AXIS RAPID). Structural parameters were refined by full-matrix least-squares (RADY) [1].

All Sr ions occupied rhombic sites. Especially, one rhombic sites had more amount of Sr ions as compared with another rhombic sites in both of the R = Sm and Nd system. These solid solutions have relationship between distribution of cations and microwave dielectric properties [2]. Therefore, improvement of these properties with increasing composition α is lead by substituting Sr ions for Ba ions.

[1] Sasaki S., *XL Report*, *ESS*, *State University of New York*, 1982, 1–17. [2] Ohsato H., *J. Eur. Ceram. Soc.*, 2001, **21**, 2703–2711.

Keywords: tungsten bronze, microwave absorption material, structure-properties relationship in solids

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Structural Investigation of Cyclamic Acid and Related Cyclamates

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There exist extensive studies on structure-taste relationship for the artificial sweetening agents, like sucralose (600 times sweeter than sucrose), saccharin (300), acesulfame-K (200) aspartame (180), and cyclamates (30). In order to perceive the sweetness, molecules must activate receptor sites in taste-bud proteins on the tongue. The activation is believed to take place when a molecule of suitable shape has a characteristic functional distribution. According to some theories, there are three essential structural components of a sweetener molecule, oriented in a triangular fashion. More elaborated theories on sweetness are given in an overview [1].

Because the shape of the molecule with the potential sweetness is important and the X-ray structural data for cyclamic acid (cyclo-hexylsulfamic acid) and cyclamates are not available, the following crystal structures were determined: cyclamic acid, sodium cyclamate, potassium cyclamate, ammonium cyclamate, rubidium cyclamate, caesium cyclamate, tetraethylammonium cyclamate, tetrapropyl-ammonium cyclamate, tetrapentylammonium cyclamate and guanidinium cyclamate.

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[1] Ellis J.W., *J. Chem. Educ.*, 1995, **72**, 671-675.

Keywords: X-ray structure, artificial sweetener, cyclamates

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Structure and Microwave Dielectric Properties on $ALa_4Ti_4O_{15}$ (A=Ba, Sr and Ca)

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Developments of microwave dielectrics for base station are desirable because of increasing amount of cellular phone. The materials are expected to have high quality factor (Q) and high dielectric constant (Σ_r). We have reported a candidate of homologous compounds Sr-doped $BaLa_4Ti_4O_{15}$ with high $Q \bullet f$ of 46000GHz, high Σ_r of 46, and a temperature coefficient of resonant frequency τ_f of -11 ppm/°C. On the other hand the τ_f can be improved to near zero: 1.3 ppm/°C with high Σ_r of 44 and $Q \bullet f$ of 47000 GHz by substituting Al ions. And when Ba ions are substituted by Sr, it also shows good: $Q \bullet f$ = 46220 GHz, Σ_r = 43.7, and τ_f = -8.4 ppm/°C. The crystal data of Ba-system are as follows: crystal system: trigonal, space group: $P\ \bar{3}c1$, and lattice constants: a =5.609 Å, c = 22.648 Å. This crystal structure belongs to hexagonal layered perovskite-type structure. The packing

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