

In our previous studies of binding properties and conformational adaptability of a known nitrate/sulfate receptor *N,N'*-3-azapentane-1,5-bis[3-(1-aminoethylidene)-6-methyl-3*H*-pyran-2,4-dione] (**L**) [4] toward various charge-dispersed monoanions ( $\text{HSO}_3^-$ ,  $\text{ClO}_4^-$ ,  $\text{IO}_4^-$ ,  $\text{PF}_6^-$  and  $\text{SbF}_6^-$ ) we have shown that **L** is able to discriminate anions on the basis of their charge density.

Herein we present two structures with the same anion,  $\text{SCN}^-$ , achieves two different complexes with **L**, thus displaying versatile binding nature of this podand. Geometry and (hydrogen-bonding) acceptor properties of  $\text{SCN}^-$  allow two distinct binding modes. When anion uses a sulfur atom as an acceptor, all strong hydrogen bond donors of the podand become coordinatively saturated by interactions with the oxo-functionalities from neighboring podands, so the only weaker C–H groups are accessible for anion binding. On the other hand, when anion uses nitrogen atom as a hydrogen-bonding acceptor then podand uses its N–H groups to accomplish optimal binding.

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**Keywords:** anion receptors, podands, binding modes

## MS74.P01

*Acta Cryst.* (2011) **A67**, C670

### Recent Advances in Two-dimensional X-ray Diffraction

Bob He, Bruker AXS, Madison, WI, (USA). E-mail: bob.he@bruker-axs.com.

The two most important developments in two-dimensional x-ray diffraction are area detectors and algorithms in analyzing 2D diffraction patterns [1]. Recent advances in area detectors, particularly the one based on the MikroGap technology, and the diffraction vector approach in 2D data analysis are discussed with experimental examples in phase identification, stress measurement, texture analysis and grain size determination.

The VÅNTEC-500 area detector, based on proprietary MikroGap technology, achieves high resolution and low detector noise with a very high dynamic range by combining the advantages of a gaseous detector with the new resistive anode micro-design. It is designed and optimized for the two-dimensional x-ray diffraction system for analytical applications in various materials research, such as nanotechnology, thin films, polymers, metals, biomaterials, forensics, and process control. The detector features a large active area and a tapered geometry which makes it possible to capture diffraction patterns in a large solid angle and to access high diffraction angles.

Two-dimensional diffraction pattern contains information in a large solid angle. The 2D image can be described by the diffraction intensity distribution in both  $2\theta$  and  $\gamma$  directions. Unit diffraction vector is used in the data analysis of the 2D diffraction pattern. The unit diffraction vector for all the pixels in the 2D pattern can be calculated in the laboratory coordinates. The data analysis requires the unit diffraction vector to be expressed in the sample coordinates, which can be obtained by vector transformation. The unit vector in the sample coordinates for Eulerian geometry are given by its three components  $\{h_1, h_2, h_3\}$ :

$$h_1 = \sin\theta(\sin\phi\sin\psi\sin\omega + \cos\phi\cos\omega) + \cos\theta\cos\gamma\sin\phi\cos\psi - \cos\theta\sin\gamma(\sin\phi\sin\psi\cos\omega - \cos\phi\sin\omega)$$

$$h_2 = -\sin\theta(\cos\phi\sin\psi\sin\omega - \sin\phi\cos\omega) - \cos\theta\cos\gamma\cos\phi\cos\psi + \cos\theta\sin\gamma(\cos\phi\sin\psi\cos\omega + \sin\phi\sin\omega)$$

$$h_3 = \sin\theta\cos\psi\sin\omega - \cos\theta\sin\gamma\cos\psi\cos\omega - \cos\theta\cos\gamma\sin\psi$$

The three components can then be used to derive fundamental equation for many applications or data corrections. The fundamental equation for stress analysis, for instance, is given by the scalar product of the strain tensor  $\epsilon_{ij}$  with the unit vector components  $\{h_1, h_2, h_3\}$ :

$$\epsilon_{(\gamma,\omega,\psi,\phi)}^{\{hkl\}} = \epsilon_{ij} \cdot h_i \cdot h_j$$

where  $\epsilon_{(\gamma,\omega,\psi,\phi)}^{\{hkl\}}$  is the measured strain at the Eulerian angles  $\omega$ ,  $\psi$  and  $\phi$ , and on the portion of the diffraction ring given by  $\gamma$ .

For texture analysis, the pole figure angles ( $\alpha, \beta$ ) are given by pole mapping equations:

The diffraction unit vector is also used in polarization correction, absorption correction and effective volume calculation for crystal size evaluation by  $\gamma$ -profile analysis.

[1] B. He, *Two-dimensional X-ray Diffraction*, John Wiley & Sons, 2009.

**Keywords:** area detector, stress, texture

## MS74.P02

*Acta Cryst.* (2011) **A67**, C670–C671

### Nullification of extinction effects in XRD analysis

I. Tomov, S. Vassilev, *Institute of Optical Materials and Technologies, Bulgarian Academy of Sciences, Acad. G. Bonchev St., Block 109, Sofia 1113, (Bulgaria)*. E-mail: iv\_tomov@yahoo.co.uk.

Based on the different behaviour of the empirical extinction coefficient  $k$  [1] and the secondary extinction (SE) coefficient  $g$  [2] with respect to the levels of interaction of the diffraction process, the present study outlines a pioneer approach to analytical nullification of the SE effects. Both the incident-beam intensity  $I_0$  and the pole density  $P$  that represent the relative volume fraction of crystallites contributing to reflection define the variation of the levels of interaction of the diffraction process. Accounting for crystal and textural anisotropy, we have shown that the above coefficients are interconnected by  $k=2g\mu/PI_0S$  or  $g=PI_0S/2k\mu$  and depend on all the parameters describing the diffraction process of a reflection, excluding only the reflectivity  $Q$ . Here,  $S$  is the cross-section of the beam, and  $\mu$  is the linear absorption coefficient. Whereas  $g$  is proportional to the product  $PI_0$ , the coefficient  $k$  is proportional to the  $g/PI_0$  ratio. Therefore, by virtue of the interdependence between  $g$  and  $PI_0$ , any change of  $P$  or  $I_0$  or both does not change the ratio  $g/PI_0$  and, hence,  $k$  is constant that is independent of the level of interaction. For a pair of levels of interaction defined by variation of incident beam intensities from  $I_{0,i}$  to  $I_{0,i^*}$ , one can show that  $k_i=k_{i^*}$ , where  $i$  and  $i^*$  denote generator current values causing the respective  $I_0$  intensity values that are related by  $I_{0,i}/I_{0,i^*}=i/i^*=R_{i,i^*}$ . Here,  $R_{i,i^*}$  is the ratio between the generator current values. The equality  $k_i=k_{i^*}$  allows analytical nullifying the SE effects by using two expressions of  $k$  defined by the intensities of a reflection measured at a series of levels of interaction. The procedure for applying this approach starts with kinematic definition of the parameter ( $R$  or  $P$ ) under study, and finishes with derivation of an operative formula for determining its extinction-free value. For the purposes of comparison, the extinction-affected pole density  $P_m$  is expressed using intensities measured at the same reflection of textured sample and powder standard. The object of this study was a nickel sample representing a moderate texture with  $\langle 100 \rangle$  preferred orientation. The results show that whereas the extinction-free values