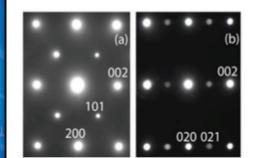
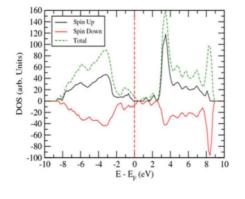


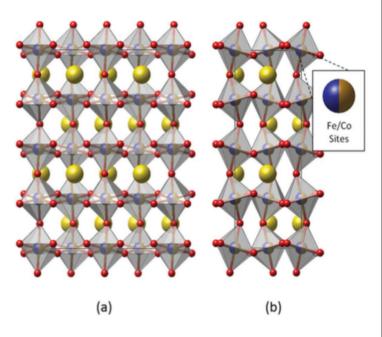
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# Powder Diffraction

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### **EDITORIAL**

Tom Blanton	Hugo Rietveld, the Person and the Method	257	
TECHNICAL ARTICLES			
<ul> <li>W. Wong-Ng, G. Liu,</li> <li>I. Levin, I. Williamson,</li> <li>P. Ackerman, K. R. Talley,</li> <li>J. Martin, K. AlHamdan,</li> <li>W. Badegaish, J. A. Kaduk</li> <li>and L. Li</li> </ul>	X-ray diffraction and density functional theory studies of $R(\text{Fe}_{0.5}\text{Co}_{0.5})\text{O}_3$ ( $R = \text{Pr}$ , Nd, Sm, Eu, Gd)	259	
Paul Angerer, Ronald Schöngrundner, Katerina Macurova, Manfred Wiessner and Jozef Keckes	Curvature determination of embedded silicon chips by <i>in situ</i> rocking curve X-ray diffraction measurements at elevated temperatures	267	
James A. Kaduk, Amy M. Gindhart and Thomas N. Blanton	Crystal structure of norgestimate, C <sub>23</sub> H <sub>31</sub> NO <sub>3</sub>	274	
G. Liu, W. Wong-Ng and J. A. Kaduk	Crystal chemistry and X-ray diffraction patterns for $Co(Ni_xZn_{1-x})Nb_4O_{12}$ ( <i>x</i> = 0.2, 0.4, 0.6, 0.8)	279	
NEW DIFFRACTION DATA			
K. Yadagiri and R. Nithya	Synthesis and crystal structure refinement of new perovskite oxides, $Dy_{0.55}Sr_{0.45}Mn_{1-x}Fe_xO_3$ ( <i>x</i> = 0.0 and 0.2) from X-ray powder diffraction data	285	
Qing Wang, Xia Zeng, Shan Shan Li, Xiao Li Ma and	X-ray powder diffraction data for 5, 6-dihydro-3-(4-morpholinyl)- 1-[4-(2-oxo-1-piperidinyl)phenyl]-2(1H)-pyridinone, $C_{20}H_{25}N_3O_3$	288	

V. D. Zhuravlev,Preparation and crystal structure of garnet-type calcium zirconium germanate292A. P. Tyutyunnik and<br/>N. I. LobachevskayaCa<sub>4</sub>ZrGe<sub>3</sub>O<sub>12</sub>292

### **DATA REPORTS**

Hui Li

Xiaoxiang Liao, Jianguo Tang, Dalin Yuan, Yanmei Huang, Hongqin Yang, Wei Zhao, Ji Yang, Ying Fan and Hui Li	X-ray powder diffraction data for menthyl lactate, $C_{13}H_{24}O_3$	295
Qiaohong Du, Qing Wang, Xinnuo Xiong, Xia Zeng and Hui Li	X-ray powder diffraction data for deferasirox, $C_{21}H_{15}N_3O_4$	298

Xiaoxiang Liao, Dalin Yuan,	X-ray powder diffraction data for monomenthyl succinate, C <sub>14</sub> H <sub>24</sub> O <sub>4</sub>	
Ying Fan, Hongqin Yang,		
Yanmei Huang, Ji Yang,		
Wei Zhao, Hui Li and		
Jianguo Tang		

301

### CORRIGENDUM

David R. Black,	Certification of standard reference material 1878b respirable	304
Marcus H. Mendenhall,	α-quartz – CORRIGENDUM	
Pamela S. Whitfield,		
Donald Windover,		
Albert Henins, James Filliben		
and James P. Cline		

### **INTERNATIONAL REPORTS**

Denise Zulli	2016 Denver X-ray Conference (DXC)	305
David Rendle	2016 British Crystallographic Association (BCA) Spring Meeting, April 4-7, 2016	308

## CALENDAR

Gang Wang	Calendar of Forthcoming Meetings	313
Gang Wang	Calendar of Short Courses & Workshops	314

# Powder Diffraction

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On the Cover: From the Technical Article "X-ray Diffraction and Density Functional Theory Studies of  $R(Fe_{0.5} Co_{0.5})O_3$  (R = Pr, Nd, Sm, Eu, Gd)" by W. Wong-Ng, et al. Clockwise from top left for the Pr compound: Electron diffraction patterns in the [100] and [001] zone axis orientations showing the presence of superlattice reflections 101 and 021 compared to the cell for cubic perovskites. The superlatticee reflections arise because of octahedral rotations. Front view and side view of the supercell with disordered B-sites. Calculated density of states show a band gap  $E_q \sim 0.43 \text{ ev}$ .

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# **Benchtop XRD for non-destructive** fossil identification of ammonites



Fossils of an extinct nautilus-like marine mollusk are commonly known as ammonites. The name is believed to be derived from their spiral shape, which resemble the Egytpian god Ammon's hat made from a ram's horn. Figure 1 shows an ammonite fossil.

Ammonites show a vast diversity of shapes, styles and colors. Classifications are based on structures of the spiral or coiled chambers, called camerae, and exterior features. The different shapes and features seem to be characteristic of different time periods. This is of great importance as the presence of a specific order or suborder in sediments can be used as a biological marker of different geological time periods by paleontologists. Figure 2 shows a white ammonite in a sample holder mounted in the MiniFlex benchtop X-ray diffractometer.

The MiniFlex can be used as a non-destructive method to determine the phase composition of the ammonites and surrounding sediments of ammonite fossils. Figure 3 shows a diffraction pattern from the MiniFlex and the observed phases that were obtained after matching the pattern to the ICDD diffraction database. The fossil can be seen to be a complex mixture of a number of carbonate, oxide, and silicate phases.





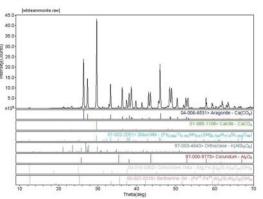


Figure 3

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MiniFlex 600





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