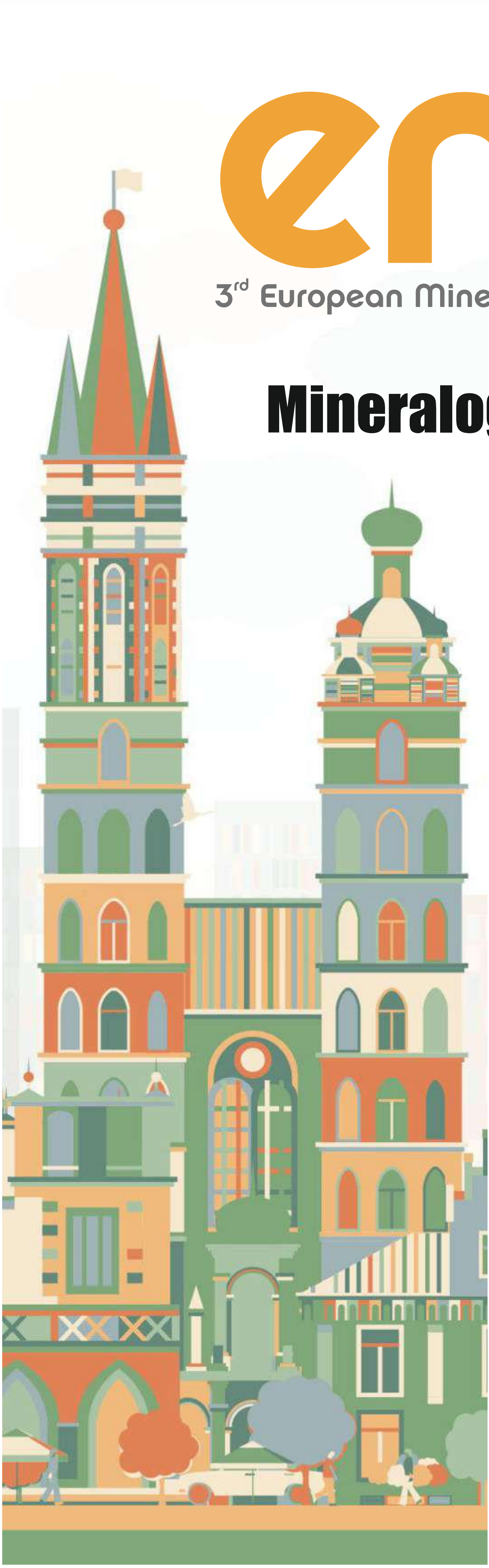
emc^{2}020

3rd European Mineralogical Conference Cracow Poland

Mineralogy in the modern world



ABSTRACT BOOK

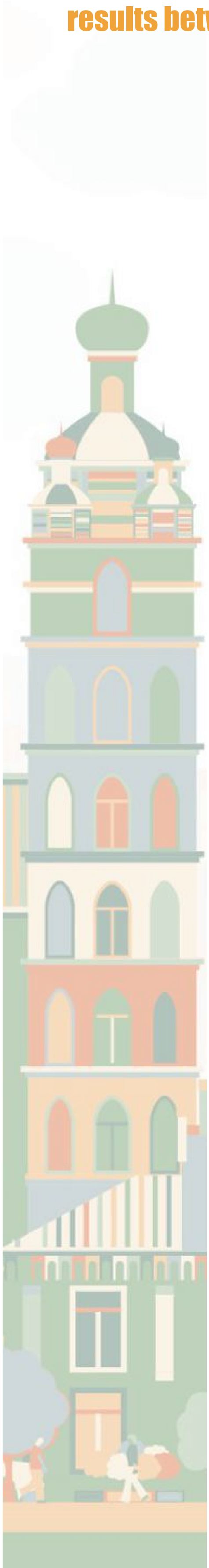
29 August - 2 September 2021

PROGRAMME

	oral blocks	STAGE 1 (Main Stage)	STAGE 2	STAGE 3	STAGE 4
Monday 30th Aug 2021	9:30 – 11:15	T1_S2	T5_S3+T11_S1	T2_S1	T8_S1+T8_S2
	11:30 – 13:00				
	15:00 – 17:15		T3_S1		
Tuesday 31th Aug 2021	9:30 -11:15	T1_S2	T10_S2+T10_S3+T10_S4 +T10_S5	T5_S1+T7_S1	T10_S1
	11:30 – 13:00	T1_S3+ T1_S4			
	15:00 – 17:15		T6_S1	T4_S1	T12_S1
Wednesday 1st Sept 2021	9:30 -11:15	T1_S5	T13_S1+T15_S1	T5_S2	T11_S2
	11:30 – 13:00			T12_S2+T12_S3 +T12_S4	
	15:00 – 17:15	T1_S1	T14_S2		
Thursday 2nd Sept 2021	9:30 -11:15	T9_S1+T9_S2	T14-S1+T16_S1	T5_S4	T11_S3+T11_S4
	11:30 – 13:00				

Mineralogy in the modern world

Following the success of the 1st and 2nd European Mineralogical Conference, the emc2020 will be focused on current and future challenges in the Earth, planetary and environmental sciences, and fostering an exchange of new views and research results between scientists from Europe and beyond.



The city of Kraków is a vibrant, academic and tourist city in the heart of Europe. Modern infrastructure, efficient public transportation and famous Polish hospitality make it a safe and friendly place for visitors from all over the world. The city dates back to Middle Ages and has traditionally been one of the leading centers of Polish and European academic, cultural, and artistic life. It was the capital of Poland from 1038 to 1569.

Welcome in Cracow!

Krakau, ክራኮው, Cracow, Cracovia, Краков, 克拉科夫, Cracó, Kraká, クラクフ, كراكوف, Cracovie, Krakov, Краків, Cra-cốp, Krakovja

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The EMC2020 is organized by the PTMin (Mineralogical Society of Poland) on behalf of other European mineralogical societies:

DMG – Deutsche Mineralogische Gesellschaft
MinSoc – Mineralogical Society of Great Britain & Ireland
MinSocFin – Mineralogical Society of Finland
ÖMG – Österreichische Mineralogische Gesellschaft
RMS – Russian Mineralogical Society
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SFMC – Société Française de Minéralogie et de Cristallographie
SIMP – Societa' Italiana di Mineralogia e Petrologia
SSMP – Swiss Society of Mineralogy and Petrology

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PRESSURE-DRIVEN METHANOL INTRUSION IN MFI-ZEOLITES AND ITS EFFECTS ON THE STRUCTURAL DEFORMATION IN SILICALITE-1

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MFI-zeolites are nowadays used in methanol-to-olefins (MTO) production processes as catalysts, representing an alternative to the high-energy demanding Steam Cracking process, which accounts for 95% of the worldwide olefins production. At ambient conditions, only the grain surfaces of the zeolite are supposed to be active in the MTO process. Applying hydrostatic pressure, the methanol molecules may be injected into the structural channels of the zeolites. The structure of MFI-zeolites is characterized by SiO4 interconnected tetrahedra, which define two major structural channels systems, confined by 10-members rings (10mR) of tetrahedra running along [010] and sinusoidal cavities along the [100] direction; minor rings, constituted by 6mR and 5mR units are also present. Comboni et al. (2020 Catalysis Today, 345, 88-96) studied, through in situ synchrotron X-ray powder diffraction, the capability of pressure to improve the methanol absorption process. In order to evaluate the magnitude of the methanol HP-driven injection process, also the intrinsic compressional behavior of silicalite-1 has been studied, using a non-penetrating pressure-transmitting fluid (i.e. silicone oil). A different compressional behavior characterizes the methanol and the silicone-oil ramps (hereafter, Sil-meth and Sil-soil), as a consequence of the intrusion of methanol within the silicalite-1 structural channels. Since no structural refinement was possible based on XRD data, we aim to define the framework deformation and methanol intrusion of silicalite-1 at varying pressure, through template-based geometric modeling, conducted on both Sil-meth and Sil-soil. This modeling identifies the flexibility intrinsic to the geometry and topology of the crystal structure, considered as a mechanical framework. Concerning the compression along the three principal crystallographic axes in Sil-meth, it has been observed that along the a- and the b-axis the structure behaves similarly, whereas along the c-axis, which does not correspond to any of the channel development directions, the structure shows a higher compression. Conversely, the Sil-soil ramp presents a more isotropic compression. As expected, the 10mR's are clearly more compressible in Sil-soil, whereas in the Sil-meth ramp the intrusion of methanol leads to the phenomenon known as "pillar effect". As pointed out by Comboni et al. (2020) for both the P-ramps, a phase transition from monoclinic to orthorhombic (MOPT) occurs at about 0.5 GPa. Although the phase transition does not largely affect the unit-cell volume of silicalite-1, in both the Sil-soil and the Sil-meth, it strongly influences the behavior of the channels under HP, changing their compressional trend at 0.5 GPa. Lastly, the behavior of the Sil-soil is characterized by a "distributed" compression, which results in a rather equal magnitude of the compression of the 10mR, 6mR, and 5mR units. Conversely, in the Sil-meth, the compression of the 10mR is significantly modest, whereas takes place a clear distortion of the 5mR units, which small diameter does not allow any methanol intrusion process.