

JANA2020 Workshop @ MLZ

Report of Contributions

Contribution ID: 1

Type: **not specified**

Welcome & Organisational details

Wednesday 18 October 2023 09:00 (10 minutes)

Session Classification: Day 1

Contribution ID: 2

Type: **not specified**

Dr. M. Dušek –Introduction to Jana2020

Wednesday 18 October 2023 09:10 (50 minutes)

Session Classification: Day 1

Contribution ID: 3

Type: **not specified**

Hands-on tutorial „First steps with Jana2020“

Wednesday 18 October 2023 10:30 (2 hours)

Example 01.1: Zn | Solution of a simple crystal structure from single crystal data

Example 02.1.1: PbSO₄ | Simple inorganic structure from powder

Session Classification: Day 1

Contribution ID: 5

Type: **not specified**

Dr. M. Henriques –Magnetic structures in Jana2020

Wednesday 18 October 2023 13:30 (1 hour)

Session Classification: Day 1

Contribution ID: 6

Type: **not specified**

Hands-on tutorial „Magnetic structures, Part 1“

Wednesday 18 October 2023 14:30 (1 hour)

Example 12.1: Ba₅Co₅ | powder data, k=0

Example 12.2: Ba₆Co₆ | powder data, k=(0,0,1/2)

Example 12.1: Ba₅Co₅ | Jana2020 –ISODISTORT communication

Example 12.5: HoNi | single crystal data, k=(0,0,1)

Session Classification: Day 1

Contribution ID: 7

Type: **not specified**

Hands-on tutorial „Magnetic structures, Part 1 “(continuation)

Wednesday 18 October 2023 16:00 (1h 30m)

Example 12.1: Ba₅Co₅ | powder data, $k=0$

Example 12.2: Ba₆Co₆ | powder data, $k=(0,0,1/2)$

Example 12.1: Ba₅Co₅ | Jana2020 –ISODISTORT communication

Example 12.5: HoNi | single crystal data, $k=(0,0,1)$

Session Classification: Day 1

Contribution ID: 8

Type: **not specified**

Dr. V. Petricek –Introduction to modulated structures

Thursday 19 October 2023 09:00 (1 hour)

Session Classification: Day 2

Contribution ID: 9

Type: **not specified**

Hands-on tutorial „First steps with modulated structures“

Thursday 19 October 2023 10:00 (1 hour)

Example 5.2: Na₂CO₃ | Simple incommensurately modulated structure from single crystal data

Example xxx –commensurate Na₂CO₃

Session Classification: Day 2

Contribution ID: **10**

Type: **not specified**

Hands-on tutorial „First steps with modulated structures“ (continued)

Thursday 19 October 2023 11:30 (1 hour)

Example 5.2: Na₂CO₃ | Simple incommensurately modulated structure from single crystal data

Example xxx –commensurate Na₂CO₃

Session Classification: Day 2

Contribution ID: **11**

Type: **not specified**

Dr. M. Henriques –magnetic symmetry in superspace

Thursday 19 October 2023 13:30 (1 hour)

Session Classification: Day 2

Contribution ID: **12**

Type: **not specified**

Hands-on tutorial „Magnetic structures, Part 2“

Thursday 19 October 2023 14:30 (1 hour)

Example 12.4: MnWO_4 | powder data, $k=(-0.209, 0.5, 0.453)$

Example 12.7: DyMn_6Ge_6 | powder data, $k_0=0$ and $k_1=(0, 0, 0.1651)$

Session Classification: Day 2

Contribution ID: **13**

Type: **not specified**

Hands-on tutorial „Magnetic structures, Part 2 “(continued)

Thursday 19 October 2023 16:00 (1 hour)

Example 12.4: MnWO_4 | powder data, $k=(-0.209, 0.5, 0.453)$

Example 12.7: DyMn_6Ge_6 | powder data, $k_0=0$ and $k_1=(0, 0, 0.1651)$

Session Classification: Day 2

Contribution ID: 14

Type: **not specified**

Dr. V. Petricek –Twinned structures in Jana2020

Friday 20 October 2023 09:00 (1 hour)

Session Classification: Day 3

Contribution ID: 15

Type: **not specified**

Hands-on tutorial „Twins“

Friday 20 October 2023 10:00 (30 minutes)

Example 3.1: AD3 –a simple pseudomerohedric twin

Example 3.3: CsLiSO₄ –a three-fold pseudomerohedric twin with unexpected unit cell

Example 07.1: Ephedrine | Commensurately modulated structure with merohedric twinning

Session Classification: Day 3

Contribution ID: **16**

Type: **not specified**

Hands-on tutorial „Twins“(continued)

Friday 20 October 2023 11:00 (1h 30m)

Example 3.1: AD3 –a simple pseudomerohedric twin

Example 3.3: CsLiSO₄ –a three-fold pseudomerohedric twin with unexpected unit cell

Example 07.1: Ephedrine | Commensurately modulated structure with merohedric twinning

Session Classification: Day 3

Contribution ID: 17

Type: **not specified**

Discussion & Wrap-up

Friday 20 October 2023 13:30 (1 hour)

Session Classification: Day 3