# Mosaicity of spin-crossover crystals

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*Material supplementary - Crystal test for the calculated Mosaicity M (see text for details) to highlight the instrumental factors*

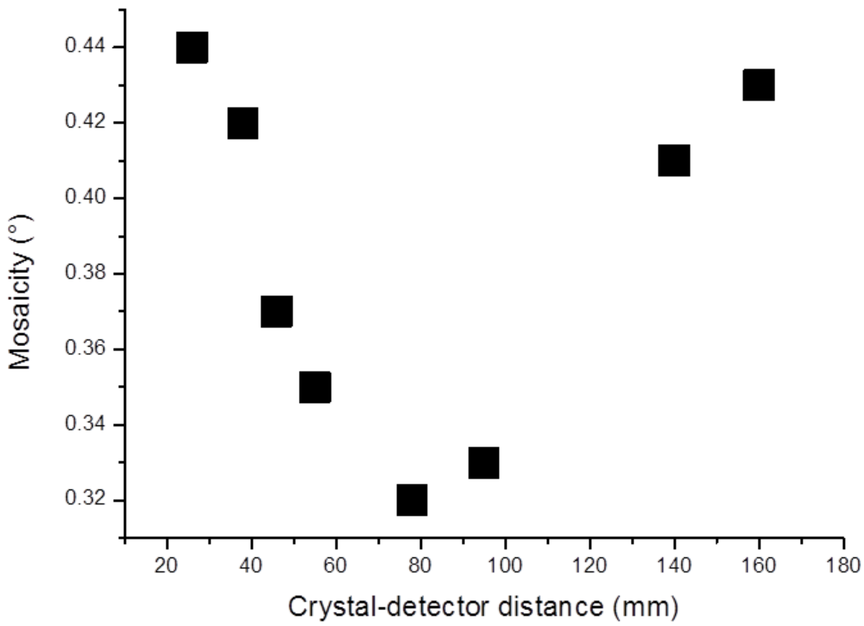


**Figure S1.** Mosaicity of the crystal test as a function of the crystal-detector distance, all other scan parameters being equal, showing a decrease followed by a strong increase at long distances. The crucial importance of the choice of this distance on the value of the mosaicity is clearly demonstrated here. The initial decrease corresponds to the fall of the number of reflexion in the data set due to the remoteness of the detector. At long distances, the mosaicity is governed by the enlargement of the Bragg peaks. For comparative purpose, similar experimental distances must be used for similar unit-cells.

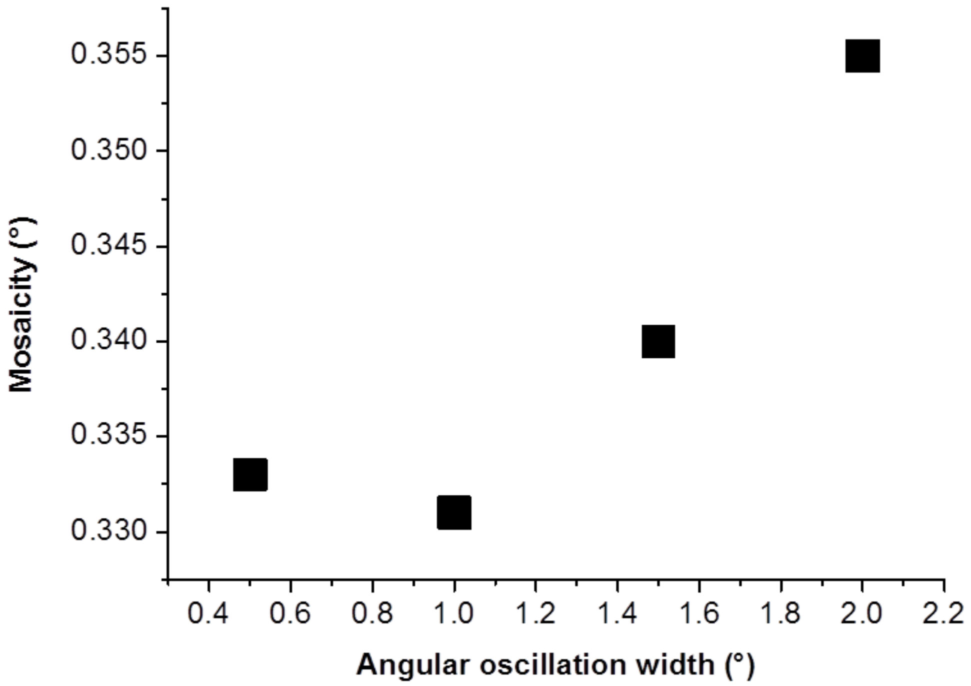


**Figure S2.** Mosaicity of the crystal test as a function of the angular oscillation width, all other scan parameters being equal, showing a strong increase for value higher than 1° that comes from a large overlap of Bragg peaks. The ideal value is sample dependent but width of about 1° should be reasonable for almost all molecular materials (unit-cell parameter mainly laying between 5 and 20 Å) - note it is the default value of many software. This figure shows the necessity to take the same value for comparative purposes.

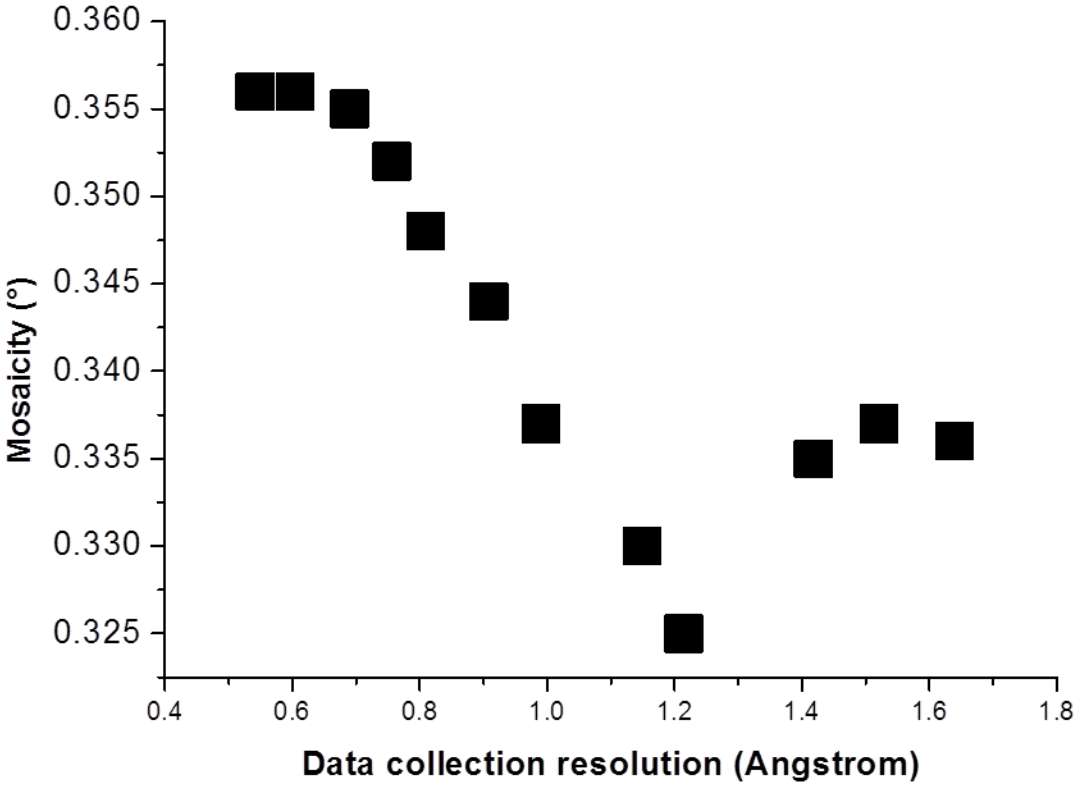


**Figure S3.** Mosaicity of the crystal test as a function of data collection resolution (Å), all other scan parameters being equal, showing a significant influence of the chosen resolution on the final value. Data collection was run with $\lambda_{Mo}$ corresponding on the above figure to theta angles from 12° to 41° (resolution from 1.64 to 0.54 Å). Standard data collection are normally run at about 0.8 Å. At low resolution, Bragg peaks (high value of the data collection resolution, small angles) are enlarged, which explains the increase of Mosaicity for values at resolution higher than 1.2 Å. The decrease from 0.7 to 1.2 Å corresponds to the decrease of the number of collected reflections when the Bragg angle increases. Standard resolution should be used for comparative purposes.

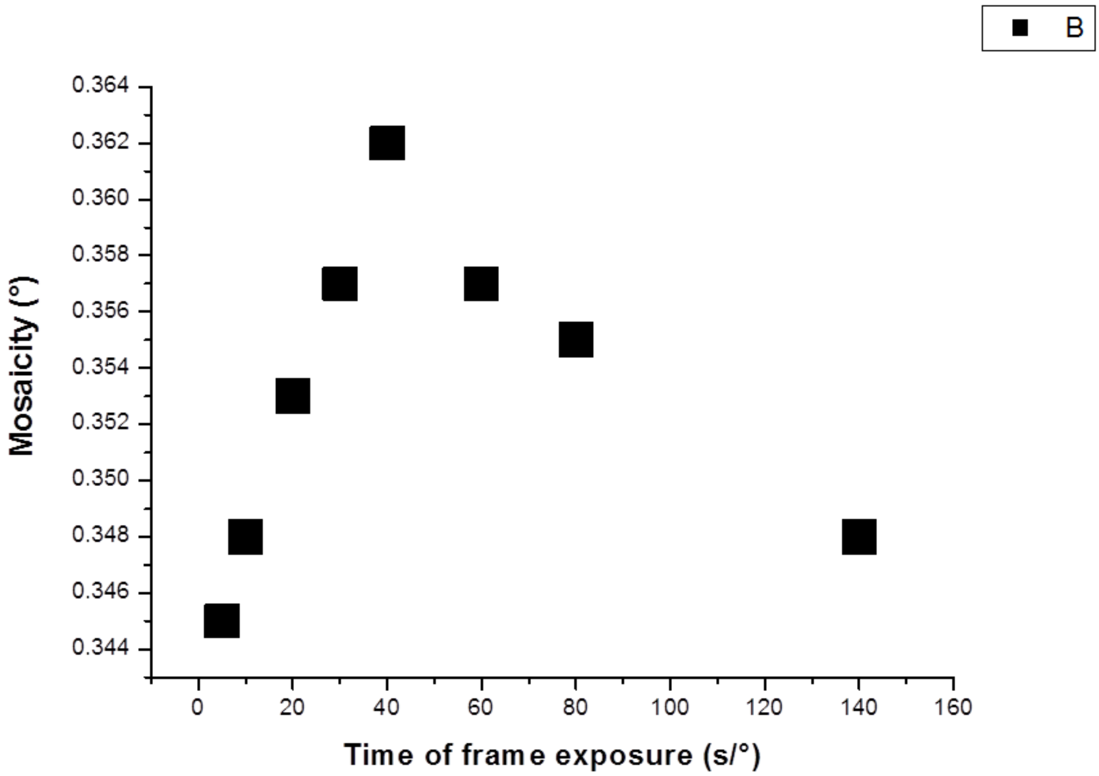


**Figure S4.** Mosaicity of the crystal test as a function of frame exposure time (s /°), all other scan parameters being equal. At short time the number of observed reflections is weaker, only more intense reflections are taken into account in that case. At long time, there is a saturation of the detection by these intense reflections corresponding to a bad Bragg peak definition. Both previous factors strongly modify the mosaicity value. As for a full data collection the time of exposure must be carefully chosen and in any cases the same must be used for comparative purposes.

| Collimator diameter (mm) | Trial 1 | Trial 2 | Trial 3 | Trial 4 |
|---|---|---|---|---|
| 0.25 | 0.34 | 0.27 | 0.25 | 0.40 |
| 0.35 | 0.375 | 0.32 | 0.28 | 0.47 |
| 0.60 | 0.38 | 0.35 | 0.30 | 0.47 |

**Table S1.** Mosaicity of the crystal test as a function of collimator diameter (mm) for four different trials corresponding to different data collection conditions (increase of the crystal detector distance from trial 1 to trial 4). The choice of the collimator, here always larger than the sample, is obviously slightly driving the calculated mosaicity value.

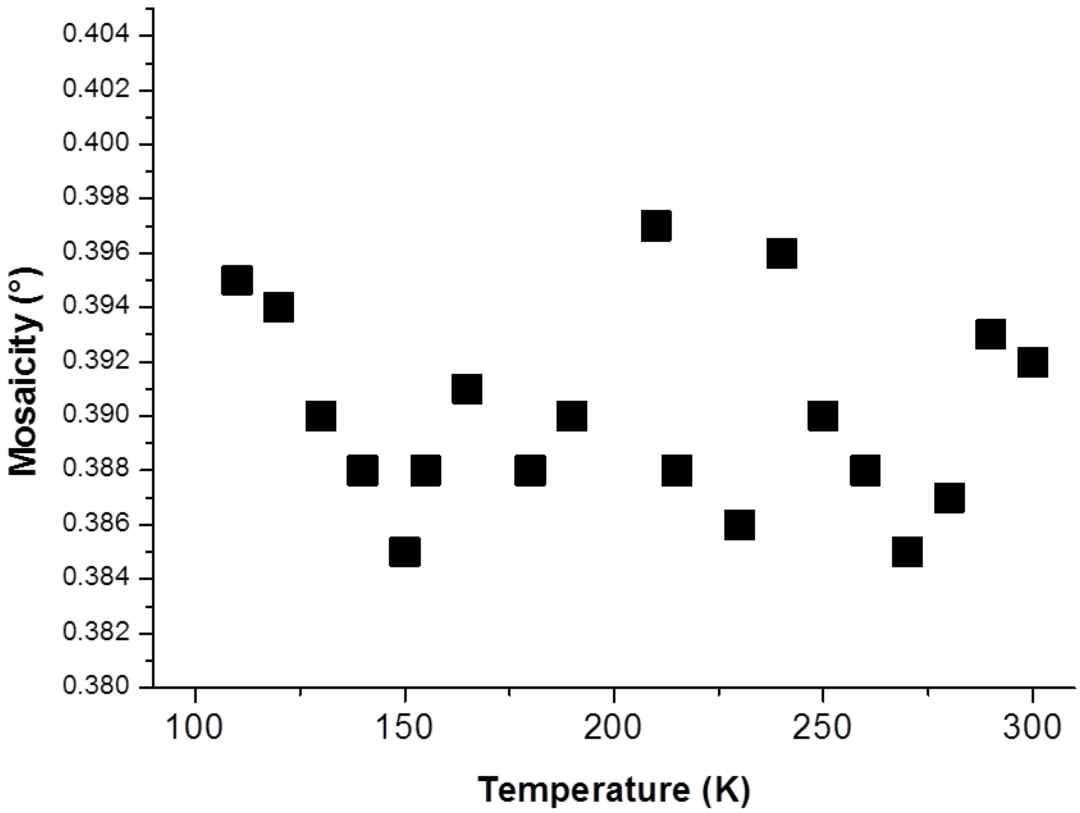


**Figure S5.** Mosaicity of the crystal test as a function of temperature, all scan parameters being strictly equal for all data collections. The influence of the temperature appears quite weak for that sample.