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**Supporting information for article:**

# Effect of synchrotron X-ray radiation damage on phase transitions in coordination polymers at high pressure

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## Supporting Information

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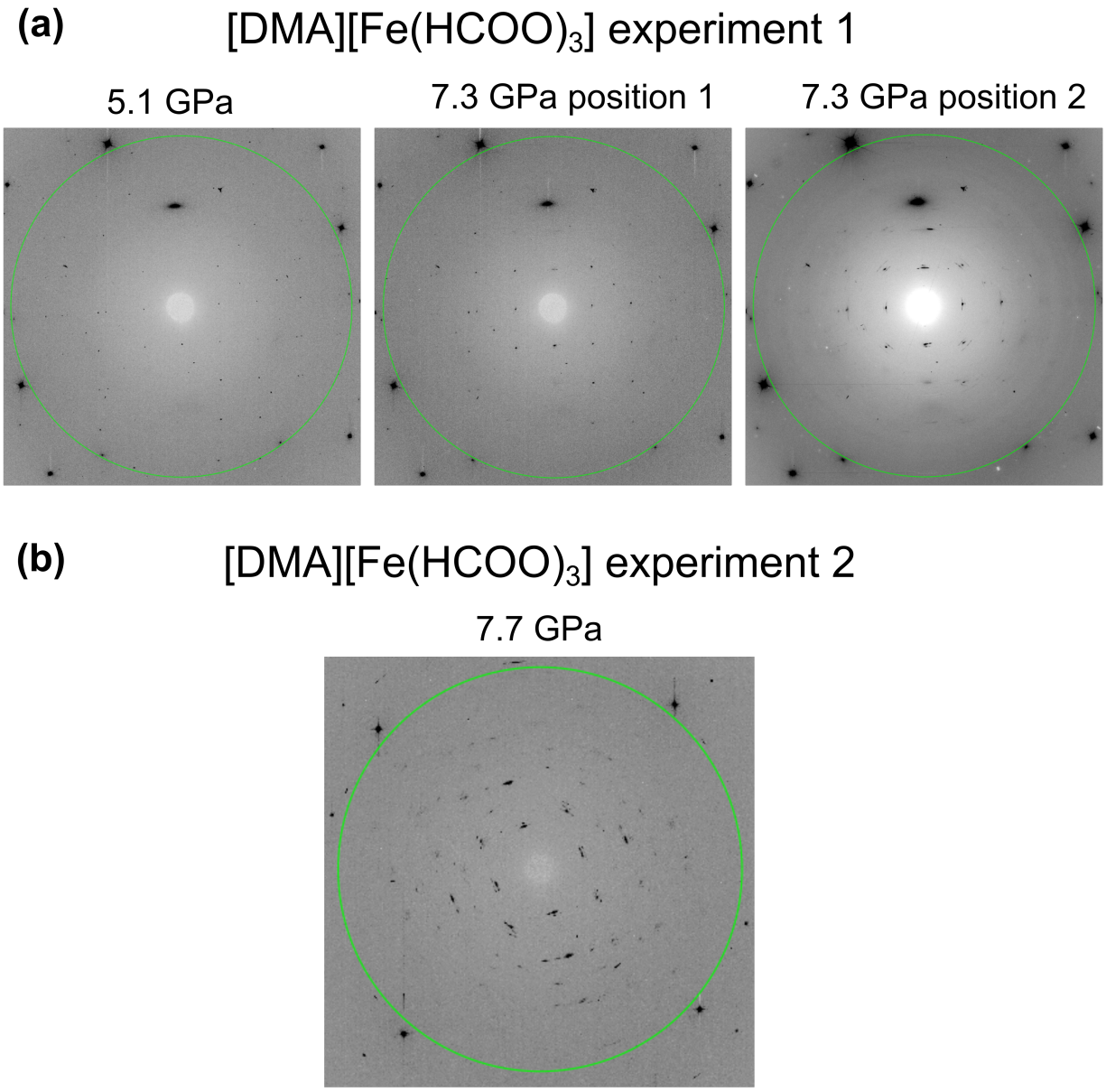


Figure S1: (a) Wide-rotation images before and after the phase transition of $[DMA][Fe(HCOO)_3]$ in experiment 1 with the green circle indicating 18 degrees $2\theta$ ($d$ = 1.3 Å) from the Dioptas interface.[S1] The 7.3 GPa pressure point indicates very weak reflections from the high-pressure phase when measured on a different position (2) to the central position 1 of the same crystal. (b) Wide-rotation image of $[DMA][Fe(HCOO)_3]$ crystal in experiment 2 measured directly at 7.7 GPa.

Table S1: Experimental parameters for [DMA][Fe(HCOO)$_3$] high-pressure experiments with the cumulative time and DWD determined up until the phase transition at 7.2 GPa. The beam size used was 10×10$\mu$m for experiments (exp.) 1 and 2, and 30×30$\mu$m for experiments 3 and 4. The beam flux could not be estimated for experiments 1 and 2 that were measured on ID09A (previous station of ID15B) at the ESRF.

| Exp. | crystal | size ($\mu$m) | Average Flux (ph/s) | Cumulative exposure time (s) | Cumulative DWD (MGy) |
|---|---|---|---|---|---|
| 1 | c1 | 20×15×10 | | 956 | |
| 2 | c1 | 35×35×20 | | 4 | |
| 3 | c1 | 95×30×30 | $4.08\times10^9$ | 786 | 0.72 |
| 3 | c2 | 45×35×20 | $4.13\times10^9$ | 914 | 0.88 |
| 4 | c6 | 70×40×30 | $3.92\times10^9$ | 310 | 0.25 |
| 4 | c7 | 40×30×15 | $2.73\times10^9$ | 154 | 0.11 |
| 4 | c8 | 40×30×20 | $5.12\times10^9$ | 154 | 0.20 |

Table S2: Experimental parameters for [DMA][Cu(HCOO)$_3$] high-pressure experiments. The beam size used was 30×30$\mu$m.

| crystal | size ($\mu$m) | Average Flux (ph/s) | Cumulative exposure time (s) at 5.4 GPa | Cumulative DWD (MGy) at 5.4 GPa |
|---|---|---|---|---|
| c1 | 30×20×15 | $4.64\times10^9$ | 1472 | 3.1 |
| c2 | 70×45×20 | $3.52\times10^9$ | 440 | 0.5 |
| c3 | 30×30×15 | $3.92\times10^9$ | 292 | 0.5 |

Table S3: Experimental parameters for Mn[Co(CN)$_6$]$_{2/3}\cdot x$H$_2$O high-pressure experiments. The flux and DWD were not calculated for c4 since the crystal fragmented upon pressure increase. The beam size used was 30×30$\mu$m.

| crystal | size ($\mu$m) | Average Flux (ph/s) | Cumulative exposure time (s) at 1.7 GPa | Cumulative DWD (MGy) at 1.7 GPa |
|---|---|---|---|---|
| c2 | 90×60×40 | $2.55\times10^{11}$ | 628 | 12.3 |
| c3 | 70×50×20 | $1.27\times10^{10}$ | 162 | 1.0 |
| c4 | 50×50×50 | | | |
| c5 | 50×50×30 | $1.27\times10^{10}$ | 156 | 0.7 |

Table S4: Experimental parameters for $Cu[Pt(CN)_6]\cdot xH_2O$ high-pressure experiments. Experiment 2 is split into the measurements in the centre of the sample (2 centre) and at different pristine positions on the sample (2 pristine), and within two pressure ranges (0–1.25 GPa and 1.4–2.5 GPa) where different photon fluxes were employed. The beam size used was $30\times30\mu$m.

| Experiment | size ($\mu$m) | Average Flux (ph/s) | Cumulative exposure time (s) | Cumulative DWD (MGy) |
|---|---|---|---|---|
| 1 | $160\times120\times30$ | $2.55\times10^{11}$ | 1 | 0.33 |
| 1 | $160\times120\times30$ | $2.55\times10^{11}$ | 4 | 1.33 |
| 2 centre | $160\times120\times30$ | $2.61\times10^{10}$ | 15 | 0.5 |
| 2 pristine | $160\times120\times30$ | $2.61\times10^{10}$ | 2 | 0.07 |
| 2 centre | $160\times120\times30$ | $2.55\times10^{11}$ | 10 | 3.3 |
| 2 pristine | $160\times120\times30$ | $2.55\times10^{11}$ | 2 | 0.7 |

Example RADDOSE-3D input for the [DMA][$Fe(HCOO)_3$] c6 crystal.

| | |
|---|---|
| # Crystal Block # | |
| Crystal | |
| Type | Cuboid |
| Dimensions | 70 40 30 |
| PixelsPerMicron | 0.5 |
| AbsCoefCalc | Smallmole |
| UnitCell | 8.25785 8.25785 22.5102 90 90 120 |
| Smallmoleatoms | C 5 H 11 Fe 1 N 1 O 6 |
| NumMonomers | 6 |
| Goniometeraxis | 0 |
| Containermaterialtype elemental | |
| Materialelements | C 1 |
| Ccontainerthickness | 1950 |
| Containerdensity | 3.5 |
| # Beam Block # | |
| Beam | |
| Type | Gaussian |
| Flux | 3.92$e$9 |
| FWHM | 30 30 |
| Energy | 30 |
| Collimation Circular | 60 60 |
| # Wedge Block # | |
| Wedge | −38 38 |
| ExposureTime | 310 |
| AngularResolution | 0.5 |

# References

(S1) Prescher, C.; Prakapenka, V. B. *High Pressure Res.* **2015**, *35*, 223–230.