MS46-1-1 Tensor of radiation expansivity – a proposed measure of structural susceptibility to radiation damage #MS46-1-1

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Abstract
The advent of fourth-generation synchrotron radiation sources of extreme brightness opens new possibilities for time resolved crystallography. However, with more routine accesses to extremely high doses of radiation during typical diffraction measurements, observable effects from radiation are increasingly observed for small molecule systems. Reproducibility and reliability of lattice parameters is of key concern for small molecule X-ray diffraction (SMX). (Christensen et al., 2019) They are commonly measured as a function of pressure and/or temperature to give thermal expansivities and bulk modulus but undetected dose effects can at best muddy the waters or at worst render these studies lacking. Negative X-ray expansion, (Coates et al., 2021) modification of polar properties, (Bogdanov et al., 2021) shift of spin equilibria in spin-crossover solids (Chernyshov et al., 2021) under irradiation serve as examples where different results might be observed as a function of energy and dose.
Here we present a set of observation of the lattice response of the radiation damage that concern dicyano-bis(triphenylphosphine)-mercury(II) [$Hg(CN)_2(PPh_3)_2$]. Repeated single crystal X-ray diffraction collections were made at fixed temperatures using synchrotron radiation on BM01, ESRF EBS. This enabled us to characterize the radiation expansivity independent of the thermal expansion.
We show that, at least in the beginning of the damage, the lattice response can be parametrized with help of a tensor, similar to the thermal expansion or compressibility. We propose that new tensorial property may serve as a measure of structural susceptibility to the radiation damage that can be spotted during a SMX experiment.

References
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