MS19 Experimental and theoretical advances in quantum crystallography

MS19-1-1 Theoretical considerations of radiation damage effects in mercury-containing compounds #MS19-1-1

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Abstract

Radiation damage in mercury compounds [1] will be examined theoretically. Since mercury (5d elements in general) has the K-edge energy levels below the energy of X-ray and usually used synchrotron radiation, absorption is a natural phenomena. This can be either manifested in higher residual densities around the heavy element atoms [2,3], or can lead to further disintegration of the crystal. Herein, we will consider the hypothesis that radiation damage is driven by a gross change of geometry of Hg containing model compounds in the excited state, which is promoted by absorption.

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References

[1] L. Bucinsky, D. Jayatilaka, S. Grabowsky. J. Phys. Chem. A 2016, 120, 6650-6669.

[2] A. Grytsiv, P. Rogl, E. Bauer, H. Michor, E. Royanian, G. Giester. Intermetallics 2010, 18, 173-178. https://doi.org/10.1016/j.intermet.2009.07.009.

[3] S. Pawlędzio, M. Malinska, M. Woińska, J. Wojciechowski, L. A. Malaspina, F. Kleemiss, S. Grabowsky K. Woźniak. IUCrJ (2021). 8, 608-620.