

## Experiment Report Form



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|   | <b>Experiment title:</b><br>Investigation of hydrogen bond symmetrization under high pressure by means of single crystal X-ray diffraction | <b>Experiment number:</b><br>HS 4723 |
| <b>Beamline:</b><br>ID15B   | <b>Date of experiment:</b><br>from: 14 Nov 2012 to: 20 Nov 2012  | <b>Date of report:</b><br>20.09.2022 |
| <b>Shifts:</b><br>12  | <b>Local contact(s):</b> Michael Hanfland  | <i>Received at ESRF:</i>             |
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### Report:

The data was published in:

Xu, W., Greenberg, E., Rozenberg, G. K., Pasternak, M. P., Bykova, E., Boffa-Ballaran, T., Dubrovinsky, L., Prakapenka, V., Hanfland, M., Vekilova, O. Y., Simak, S. I., & Abrikosov, I. A. (2013) Pressure-induced hydrogen bond symmetrization in iron oxyhydroxide. *Phys. Rev. Lett.*, 111, 175501.

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### Abstract

Under high pressures the hydrogen bonds were predicted to transform from a highly asymmetric soft O-H...O to a symmetric rigid configuration in which the proton lies midway between the two oxygen atoms. Despite four decades of research on hydroxyl containing compounds, pressure induced hydrogen bond symmetrization remains elusive. Following single crystal x-ray diffraction, Moessbauer and Raman spectroscopy measurements supported by ab initio calculations, we report the H-bonds symmetrization in iron oxyhydroxide, FeOOH, resulting from the Fe3p high-to-low spin crossover at above 45 GPa.