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Metal iodates under pressure

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Metal iodates form a diverse range of non-centrosymmetric structured materials, which exhibit useful and interesting properties such as non-linear optics; visible to far-IR transparency; large second-harmonic generation coefficients; a high optical damage threshold; and good thermal stability. They have been intensely studied under ambient conditions. In contrast, there remains a large deficit of studies of metal iodates under high-pressure (HP) conditions despite the clear possibility for new insights into pressure-induced effects, in particular changes regarding the stereochemically active lone electron pair (LEP) of the iodate ion.

During the last two years we have systematically studied different iodates using synchrotron radiation at the MSPD and MIRAS beamlines of ALBA [1-3]. Our studies have been focused in Mg(IO3)3, Zn(IO3)2, and Co(IO3)2. High-pressure synchrotron powder X-ray diffraction studies on these compounds have provided evidence of the existence of several phase transitions at relative low pressures. They have also revealed a highly anisotropic behavior. A structural analysis from experiments have shown the existence of an extremely compressible direction which coexist with a counterintuitive pressure-induced expansion along other crystallographic directions. High-pressure infrared and Raman spectroscopy have shown that there are internal modes of the iodate molecule which soften under compression. This has been related to a pressure-driven increase of the length of I–O bonds. This phenomenon is induced by the high-pressure behavior of the lone electron pairs of iodine atoms. The discovered structural changes are characterized by the increase of the oxygen coordination of the iodine atoms and the formation of up to three additional I-O bonds. Pressure–volume equations of state are presented, as well as a detailed discussion of the pressure dependences of the observed vibrational modes. With the help of DFT calculations, the results of structural studies have been used to explain changes under compression of the band-gap energy of Mg(IO3)3, Zn(IO3)2, and Co(IO3)2 which have been determined from optical-absorption measurements.

[1] A. Liang et al. Phys. Rev. B 103, 054102 (2021).
[2] A. Liang et al. J. Phys. Chem. C 125, 17448 (2021).
[3] A. Liang et al. Phys. Rev. B 105, 054105 (2022).

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