ESRF	**Experiment title:** Physical and chemical properties of Xe-O2 mixtures under pressure	**Experiment number**: HS-3829
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Names and affiliations of applicants (* indicates experimentalists):

Dewaele Agnès*, Lazicki Amy*, CEA, France

Report:

The aims of this proposal were: (1) to determine the crystallographic structure of two Xe/O2 alloys which have already been evidenced by us using Raman spectroscopy under high pressure. (2) To investigate the bond destabilization of O2 in a dense Xe environment, eventually leading to the formation of xenon oxides under ultra-high pressure.

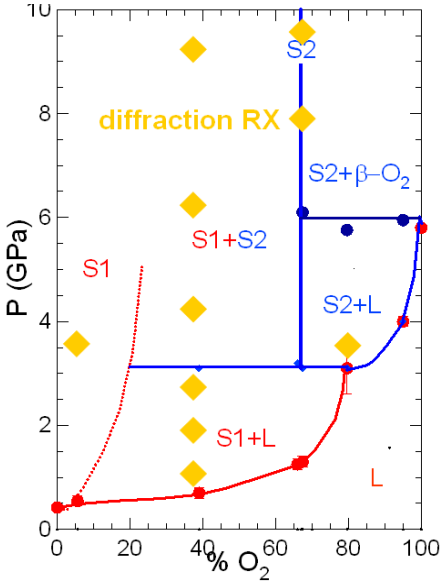

Figure 1: phase diagram of the Xe-O2 system. The yellow diamonds indicate the conditions at which X-ray diffraction data have been taken.

(1) We have determined the structure of the solids S1 and S2 previously evidenced by visual observation and Raman spectroscopy in the binary phase diagram of Xe-O2 (see figure 1). S1 is a fcc solid, with the same volume as pure xenon. S2 is a cubic Laves phase similar to MgCu2 (see figure 2). In this structure, Xenon atoms occupy the positions of Mg and O2 molecules the positions of Cu atoms. At 3.2 GPa, the pressure of formation of S2, the ratio between xenon and O2 radii is 1.17. This value is close to the ideal radio of 1.22 for the formation of Laves phase from a mixture of hard spheres with two different radii. The pressure stability field of S2 has been determined. Above 14 GPa, S2 undergoes a phase transition to a lower symmetry structure, followed by a progressive amorphization and a partial dissociation (helped by X-ray or laser irradiation) into a mixture of Xe and O2. S2 is thus metastable above 30 GPa. However, the layered

structure of S2 survives up to 100 GPa, as we could measure the (111) peak of its cubic cell up to this pressure.

These observations are published in Phys. Rev. B. (G. Weck, A. Dewaele and P. Loubeyre, “Oxygen/noble gas binary phase diagrams at 296 K and high pressure”, Phys. Rev. B 82, 0141120, 2010).

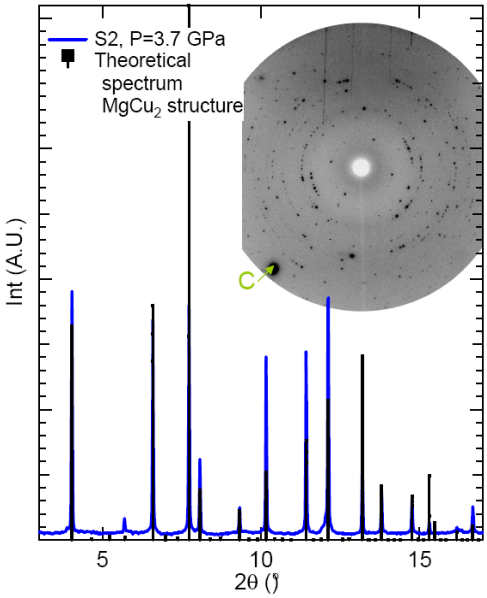

Figure 2: X-ray diffraction spectrum of S2.

(2) Starting from the compositions Xe(O2)2 and XeO2 (mixtures of S2 and S1 phases), we have obtained the same new compound by YAG laser heating above 77 GPa. The reaction was faster starting with the Xe(O2)2 mixture, which suggests that the formula of the reaction product might be close to Xe(O2)2. No detectable change of the pressure in the sample chamber was observed after reaction. The Equation of State of the reaction product was measured upon pressure decrease between 100 and 33 GPa, the pressure of its destabilization. We have further characterized the reaction product by Raman spectroscopy in our laboratory; it exhibits several Raman-active modes between 200 and 800 cm-1. These data suggest that a xenon oxide has been synthesized from a mixture of xenon and oxygen under pressure.

The nature of bounding and the properties of the product will also be determined by joined ab initio simulations and experiments.