Supporting Information for Publication High-Pressure Raman Study of $Fe(IO_3)_3$: Soft-Mode Behavior Driven by Coordination Changes of Iodine Atoms

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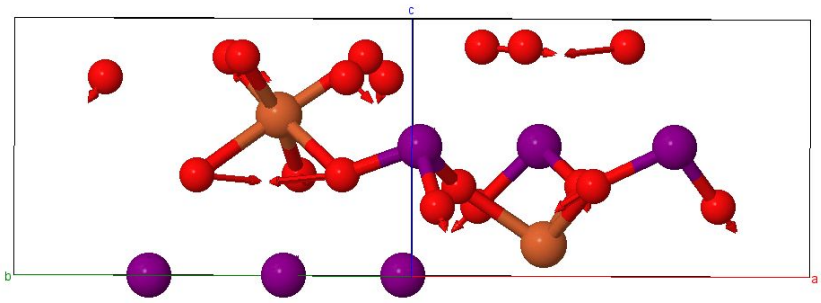

Figure S1: View of the atomic vibrations of the A^{11} mode of $Fe(IO_3)_3$ calculated at 729.2 cm^{-1} and corresponding to the experimental mode of 792 cm^{-1}. Orange, purple and red balls represent Fe, I and O atoms, respectively. This mode is a symmetric stretching I-O mode where the three O atoms of IO_3 units vibrate in-phase against the iodine atom.

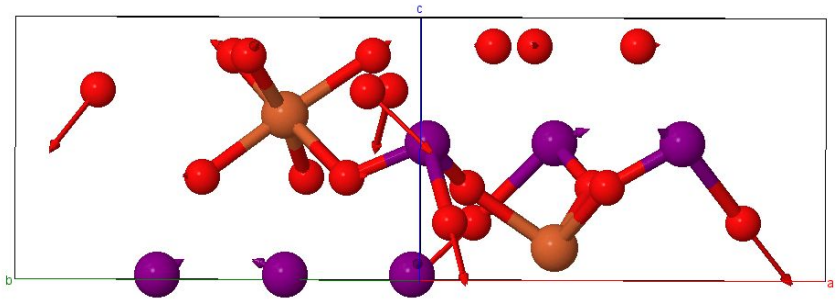

Figure S2: View of the atomic vibrations of the A^{12} mode of $Fe(IO_3)_3$ calculated at 774.0 cm^{-1} and corresponding to the experimental mode of 821 cm^{-1}. Orange, purple and red balls represent Fe, I and O atoms, respectively. This mode is an asymmetric stretching I-O mode where the one of the O atoms of IO_3 units vibrate against the iodine atom, while the other two O atoms are almost at rest.

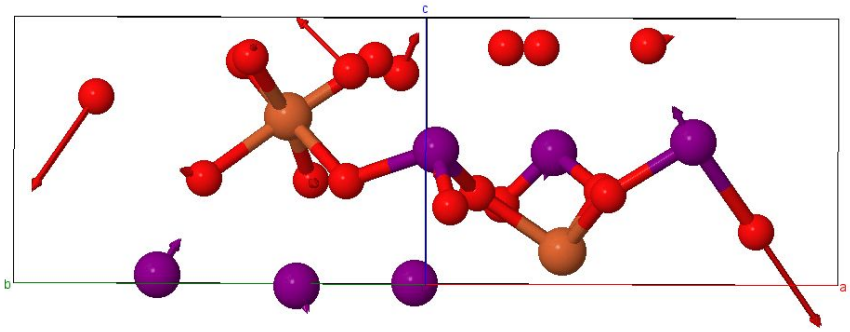

Figure S3: View of the atomic vibrations of the E_2^{13} mode of $Fe(IO_3)_3$ calculated at 791.1 cm^{-1} and corresponding to the experimental mode of 829 cm^{-1}. Orange, purple and red balls represent Fe, I and O atoms, respectively. This mode is an asymmetric stretching I-O mode where the one of the O atoms of IO_3 units vibrate against the iodine atom, while the other two O atoms are almost at rest. Note the different small movement of I atoms in this mode and in the A^{12} mode.

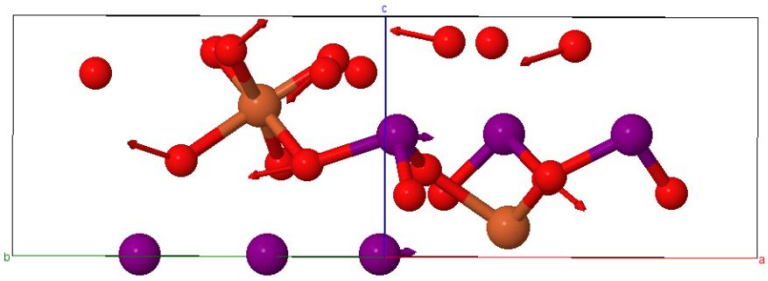

Figure S4: View of the atomic vibrations of the E_1^{10} mode of $Fe(IO_3)_3$ calculated at 622.1 cm^{-1} and corresponding to the experimental mode of 685 cm^{-1}. Orange, purple and red balls represent Fe, I and O atoms, respectively. This mode is another asymmetric stretching I-O mode where the two of the O atoms of IO_3 units vibrate out-of-phase against the I atom, while the other O atom is almost at rest.

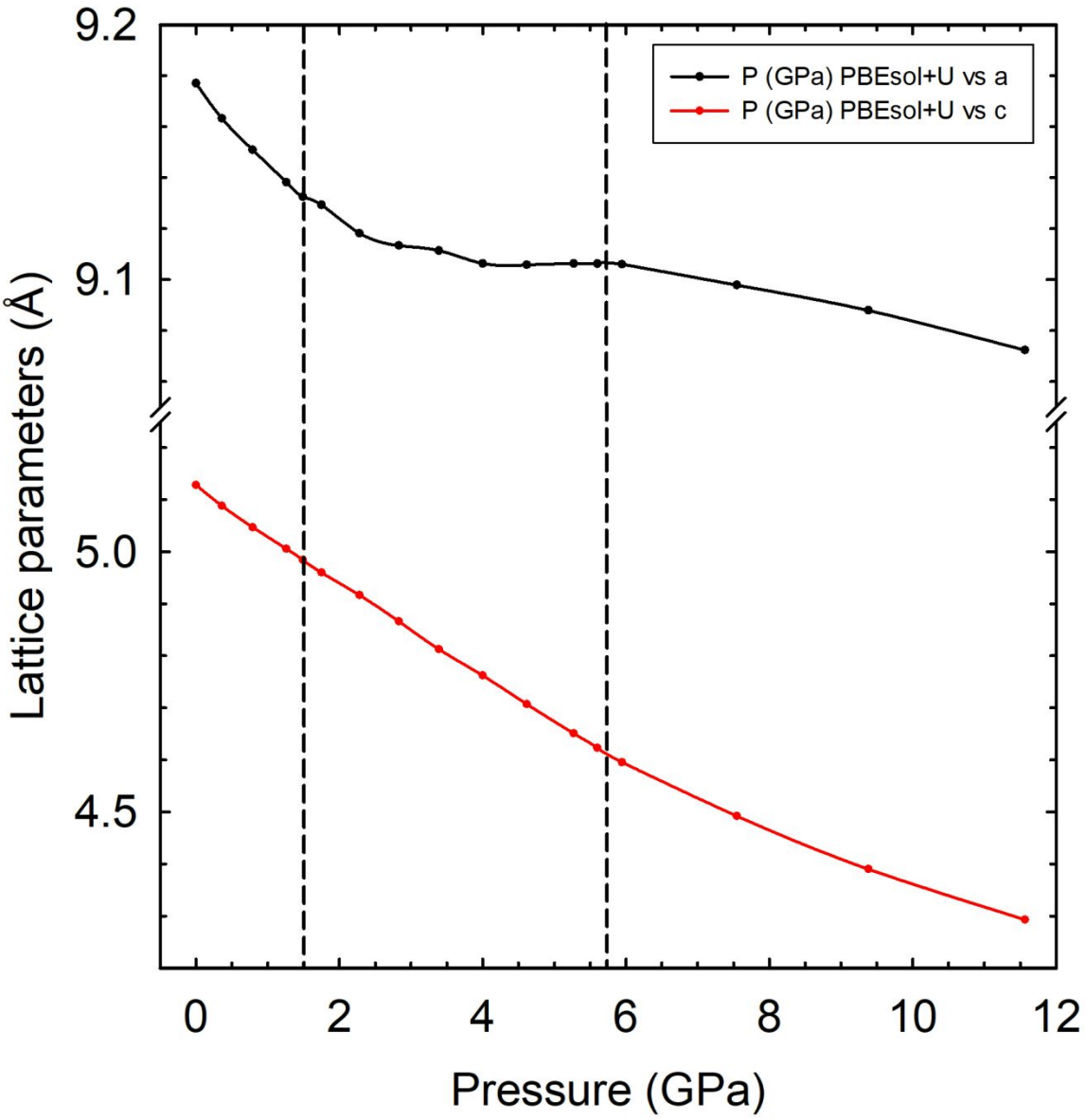

Figure S5: Calculated pressure dependence of lattice parameters a and c in $Fe(IO_3)_3$. The vertical dashed lines indicate the pressures where changes associated to the IPTs can be observed.

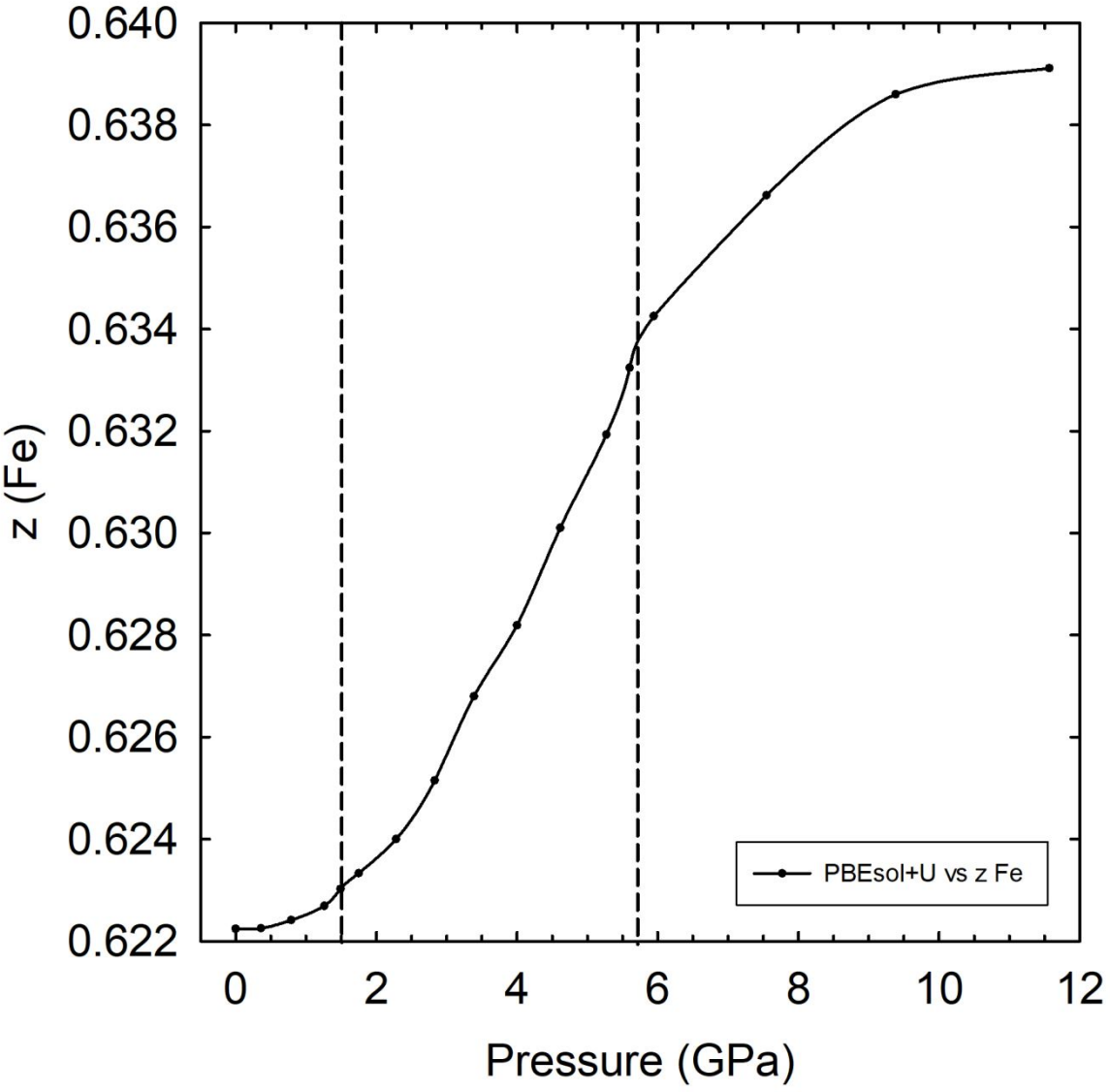

Figure S6: Calculated pressure dependence of z free atomic parameter of the Fe atom in $Fe(IO_3)_3$. The vertical dashed lines indicate the pressures where changes associated to the IPTs can be observed. Note the S-like behavior of this free atomic parameter.

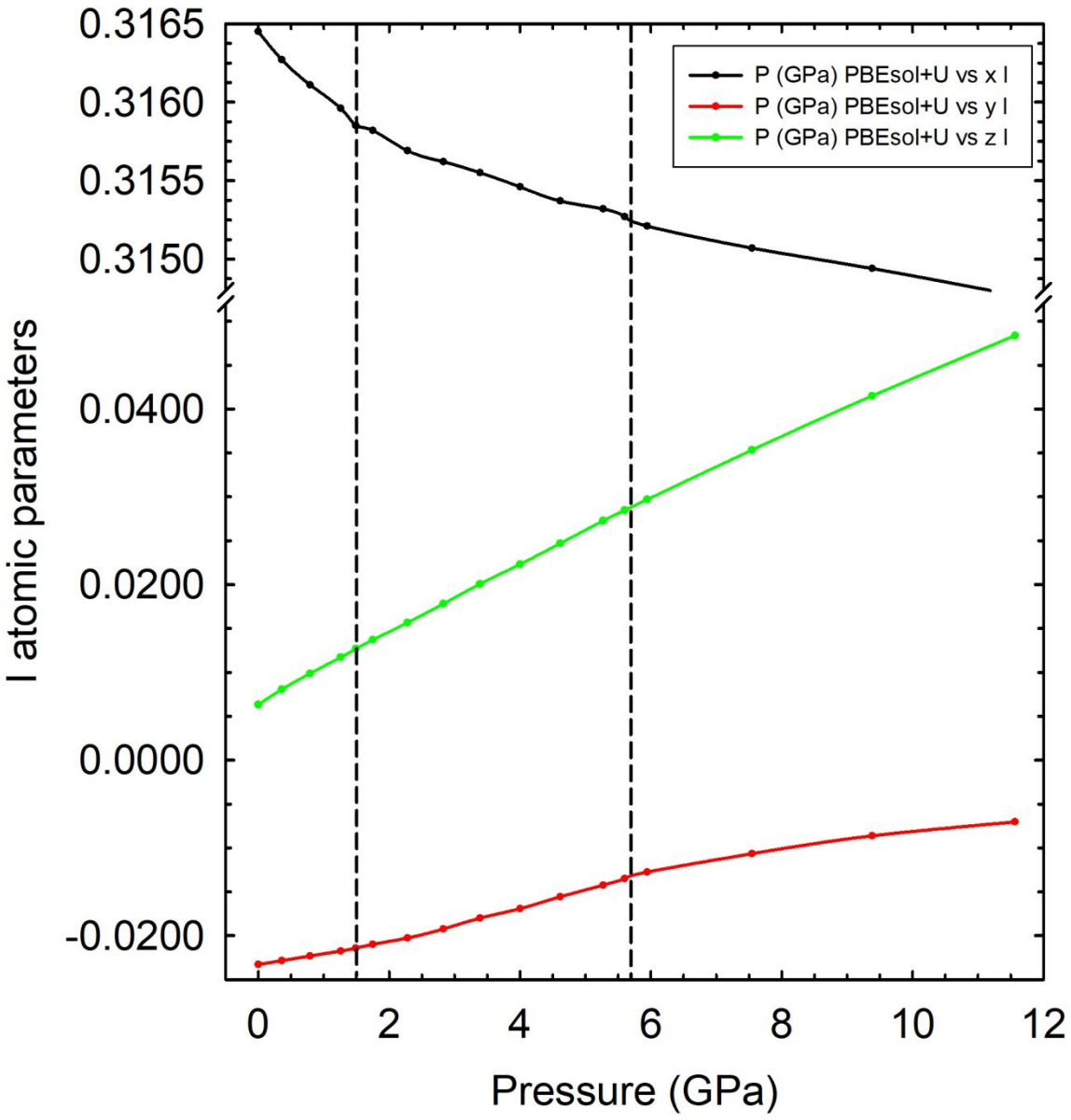

Figure S7: Calculated pressure dependence of x, y, and z free atomic parameters of the I atom in $Fe(IO_3)_3$. The vertical dashed lines indicate the pressures where changes associated to the IPTs can be observed. Note the S-like behavior of the y free atomic parameter.

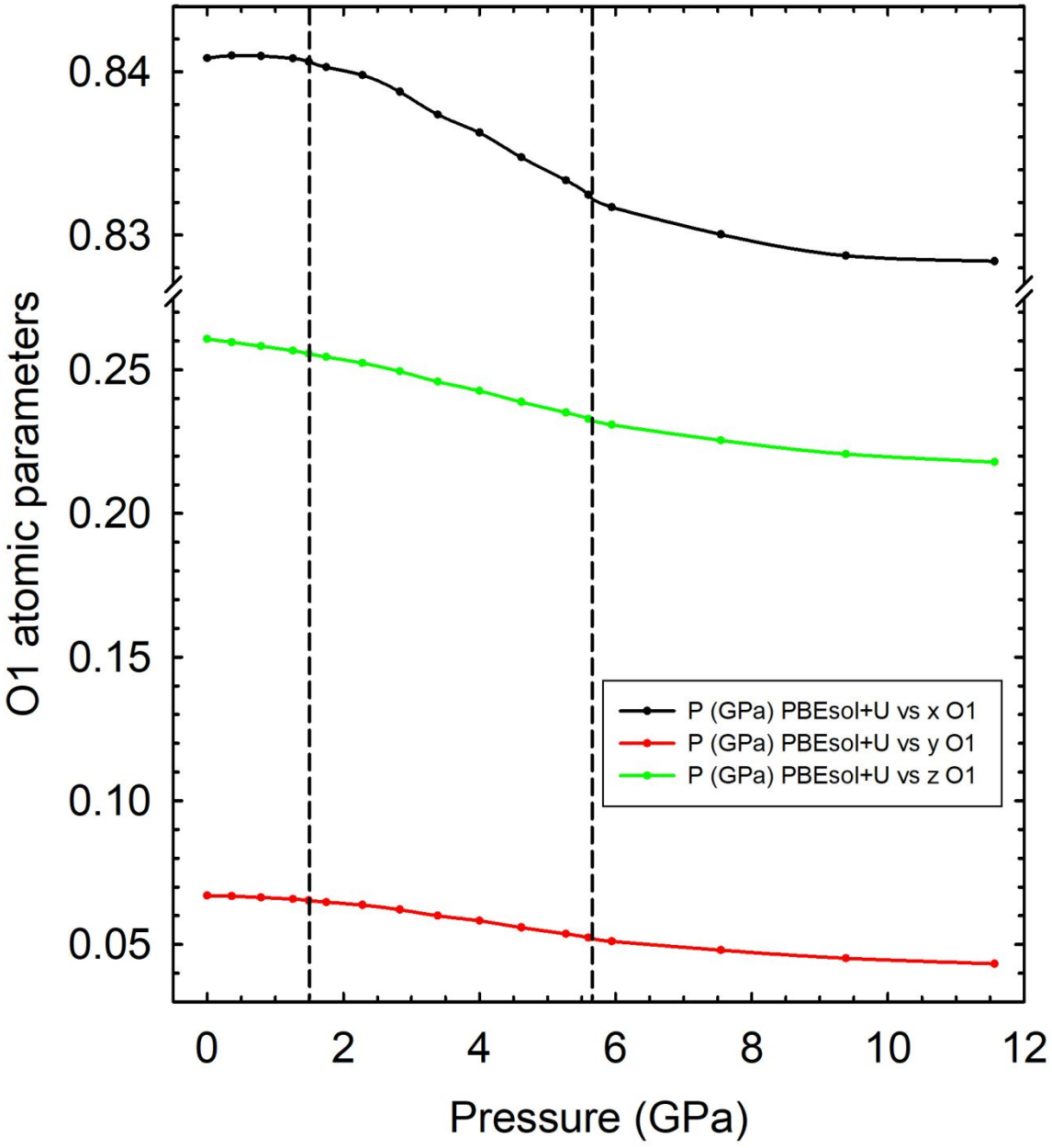

Figure S8: Calculated pressure dependence of x, y, and z free atomic parameters of the O1 atom in $Fe(IO_3)_3$. The vertical dashed lines indicate the pressures where changes associated to the IPTs can be observed. Note the S-like behavior of the three free atomic parameters.

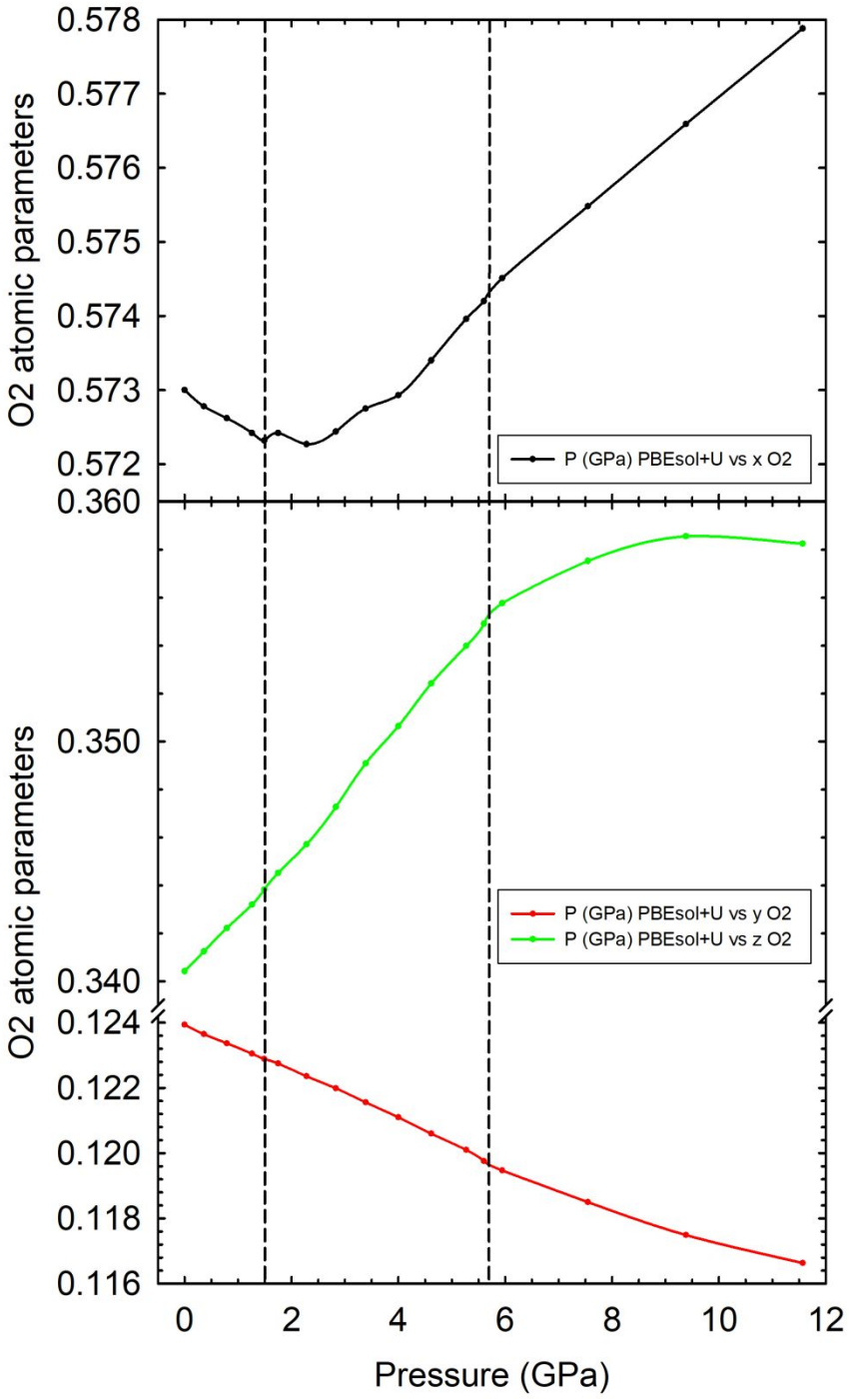

Figure S9: Calculated pressure dependence of x, y, and z free atomic parameters of the O2 atom in $Fe(IO_3)_3$. The vertical dashed lines indicate the pressures where changes associated to the IPTs can be observed. Note the completely different behavior of the three free atomic parameters in the three pressure regions.

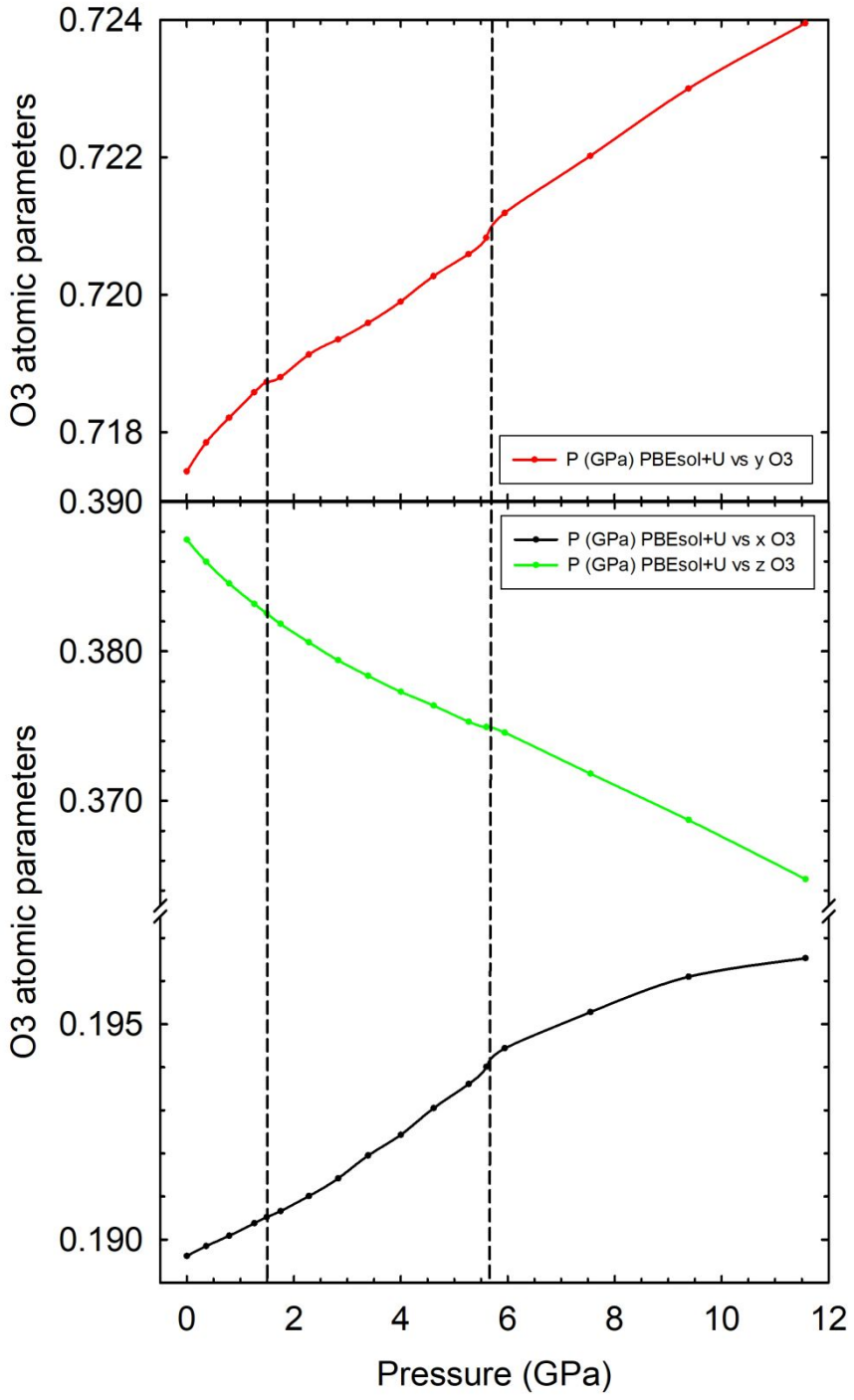

Figure S10: Calculated pressure dependence of x, y, and z free atomic parameters of the O3 atom in $Fe(IO_3)_3$. The vertical dashed lines indicate the pressures where changes associated to the IPTs can be observed. Note the completely different behavior of the three free atomic parameters in the three pressure regions.