Pressure-induced Phase Transitions and Correlation between Structure and Superconductivity in Iron-based Superconductor Ce(O$_{0.84}$F$_{0.16}$)FeAs

Jinggeng Zhao,[*,†,‡] Haozhe Liu,[*,†] Lars Ehm,[‡,¶] Dawei Dong,[#,‡] Zhiqiang Chen,[¶]

Qingqing Liu,[§] Wanzheng Hu,[§] Nanlin Wang,[§] and Changqing Jin[§]

[†]*Natural Science Research Center, Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin 150080, China*

[‡]*Photon Sciences Directorate, Brookhaven National Laboratory, Upton, New York 11973, USA*

[¶]*Mineral Physics Institute, Department of GeoScience, Stony Brook University, Stony Brook, New York 11794, USA*

[#]*Department of Physics, Harbin Institute of Technology, Harbin 150080, China*

[§]*Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

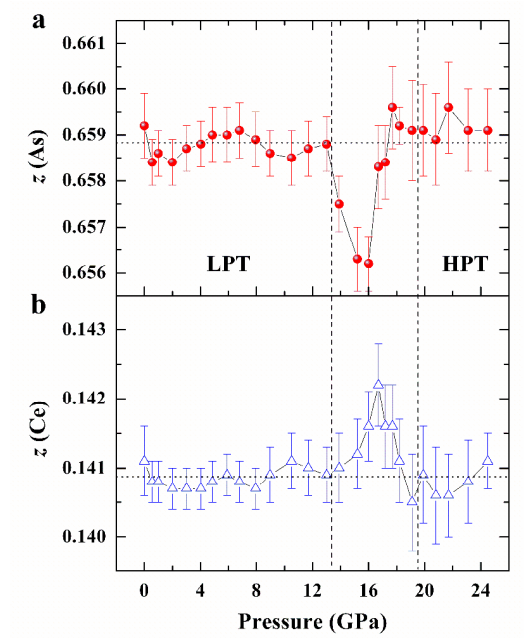E-mail: haozhe@hit.edu.cn; zhaojinggeng@gmail.com.

Figure S1. The pressure dependences of the atomic parameter z of (a) As and (b) Ce ions of $Ce(O_{0.84}F_{0.16})FeAs$.

Table S1. The summary of structure and superconductivity under high pressure for the 1111-type iron-based superconductors $Ln(O_{1-x}F_x)FeAs$ (Ln=La, Ce, Pr, Nd, Sm).

Ln	La	Ce	Pr	Nd	Sm
P_c (GPa)	No	13.9	—	9.5[15]	No
B_0 (GPa) [B_0']	78(2)[17] [7.4]	94(2) [5]	—	102(2)[15] [4]	103(1)[16] [3.1]
T_{cmax} (K)	43[23] [4 GPa]	No	—	—	55.2[26] [0.6 GPa]
P_d (GPa)	No	12.8[24]	—	—	No
r_{Ln}[42] (nm)	0.1160	0.1143	0.1126	0.1109	0.1079

Notes: P_c is the pressure for isostructural phase transition, B_0 is the ambient pressure isothermal bulk modulus for the LPT phase, T_{cmax} is the maximal superconducting transition temperature under high pressure, P_d is the pressure at the drop of T_c-P curves, r_{Ln} is the radius of Ln^{3+} ion with the coordination number of eight, and the symbol "—" indicates that no corresponding experiment results up to now.