# Experimental report

20/03/2019

**Proposal:** 5-23-707 **Council:** 4/2018

**Title:** Structure Property Relationships of the Insulator-Insulator Transition in CeMnAsO1-xFx (x = 0.00 - 0.08)

**Research area:** Chemistry

**This proposal is a new proposal**


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**Samples:** CeMnAsO
CeMnAsO0.965F0.035
CeMnAsO0.94F0.06
CeMnAsO0.925F0.075
CeMnAsO0.92F0.08
CeMnAsO0.97F0.03
CeMnAsO0.95F0.05

| Instrument | Requested days | Allocated days | From | To |
|---|---|---|---|---|
| D20 | 2 | 2 | 19/09/2018 | 21/09/2018 |
| D2B | 2 | 3 | 18/10/2018 | 21/10/2018 |


## Abstract:

CeMnAsO is a Mott insulator and an unusual insulator-insulator transition is observed at low temperature upon electron doping, by substituting F- for O2-. CeMnAsO1-xFx (x = 0 - 0.08) have been synthesised. Below the transition temperature, TII, the resistivity is observed to increase by > 3 orders of magnitude over a 5 K temperature range for CeMnAsO1-xFx (x > 0.03). The preliminary results strongly suggest that the unusual insulator-insulator transition is a result of many body localisation (MBL) of the electrons which has not been previously reported in a bulk electronic phase. The proposed MBL phase is only observed over a narrow doping range (x = 0.035 - 0.075 inclusive). We propose to investigate the electronic phase diagram of CeMnAsO1-xFx by determining if there is any correlation between TII and bond lengths/angles. We also want to verify the stoichiometry of the different phases and determine how the Mn spin transition changes with electron doping.

**Experiment 5-23-707**

**Structure Property Relationships of the Insulator-Insulator Transition in $CeMnAsO_{1-x}F_x$ (x = 0.00 - 0.075)**

CeMnAsO is a Mott insulator and an unusual insulator-insulator transition is observed at low temperature upon electron doping. Below TII the resistivity is observed to increase by > 3 orders of magnitude over a 5 K temperature range for CeMnAsO1-xFx (x > 0.03). Many body localisation (MBL) is an emergent quantum feature and is currently a subject of much debate. It is thought to arise in interacting systems where quantum mechanics overcomes the thermalisation of statistical mechanics. A notable characteristic of MBL systems is that below a transition temperature ($T_{II}$) they will become perfect insulators, exhibiting zero thermal and electrical conductivity. The $CeMnAsO_{1-x}F_x$ phases investigated so far display all of the characteristics proposed for the MBL phase such as time dependence of the MBL transition temperature and strong sensitivity of the resistivity to the applied current.

In this experiment we have investigated structure property relationships across the series $CeMnAsO_{1-x}F_x$ (x = 0.00 - 0.075). The data were recorded at 290 K on the high resolution diffractometer D2B for four hours for each sample. Preliminary results are given below:

Increasing the $F^-$ content up to 5% decreases the unit cell parameters, with the largest magnitude difference observed in the *c* parameter (**Figure 1**). In general, this can be attributed to a combination of factors, namely the thickness of the component CeO/F and MnAs tetrahedral layers in addition to the distance between these layers (interlayer spacing).

The data obtained from the neutron refinements are given in **Table 1.** The variation of the cell parameters and selected bond angles are given in **Figures 1-2**.

**Table 1:** Neutron refinement results for $CeMnAsO_{1-x}F_x$ at 300 K, including cell parameters, atomic parameters, agreement factors, and selected bond lengths and angles.

| Atom | | $CeMnAsO_{1-x}F_x$ | | | |
|---|---|---|---|---|---|
| | x = | 0.0 | 3.5 | 5.0 | 7.5 |
| Ce | z | 0.1319(2) | 0.1321(2) | 0.1326(3) | 0.1330(3) |
| | $U_{iso}$ / Å$^2$ | 0.0052(5) | 0.0047(5) | 0.0037(9) | 0.0038(8) |
| Mn | $U_{iso}$ / Å$^2$ | 0.0057(5) | 0.0070(5) | 0.0068(8) | 0.0063(7) |
| As | Occupancy | 0.972(6) | 0.987(6) | 0.976(8) | 0.984(7) |
| | z | 0.6714(2) | 0.6713(2) | 0.6718(3) | 0.6713(2) |
| | $U_{iso}$ / Å$^2$ | 0.0056(5) | 0.0058(5) | 0.0050(8) | 0.0061(7) |
| O/F | $U_{iso}$ / Å$^2$ | 0.0057(4) | 0.0052(4) | 0.0046(7) | 0.0051(6) |
| | *a* / Å | 4.09197(2) | 4.09071(5) | 4.09017(8) | 4.09107(7) |
| | *c* / Å | 8.9718(2) | 8.9675(2) | 8.9646(2) | 8.9678(2) |
| | $\chi^2$ / % | 1.31 | 1.72 | 1.13 | 1.36 |
| | $R_P$ / % | 3.37 | 3.41 | 3.30 | 3.66 |

| | | | | |
|---|---|---|---|---|
| $R_{WP}$ / % | 4.27 | 4.48 | 4.15 | 4.75 |
| V / Å$^3$ | 150.226(4) | 150.061(5) | 149.973(8) | 150.093(7) |
| Ce—O/F / Å | 2.3635(10) | 2.3636(9) | 2.3655(14) | 2.3676(12) |
| Mn—As / Å | 2.5593(10) | 2.5579(9) | 2.5603(15) | 2.5581(12) |
| Ce–O/F–Ce (1) / ° | 119.91(8) | 119.85(7) | 119.66(12) | 119.53(10) |
| Ce–O/F–Ce (2) / ° | 104.52(4) | 104.55(3) | 104.63(5) | 104.69(4) |
| Mn–As–Mn (1) / ° | 111.16(3) | 111.14(3) | 111.22(4) | 111.14(4) |
| Mn–As–Mn (2) / ° | 106.15(6) | 106.19(6) | 106.03(9) | 106.19(7) |
| Ce—As / Å | 3.3893(10) | 3.3876(9) | 3.3821(14) | 3.3838(12) |
| Mn—Mn / Å | 2.89346(2) | 2.89257(8) | 2.89219(11) | 2.89282(10) |
| MnAs layer / Å | 3.07498(191) | 3.07197(179) | 3.08062(277) | 3.07226(232) |
| CeO/F layer / Å | 2.36669(251) | 2.36897(230) | 2.37758(358) | 2.38453(296) |
| Interlayer spacing / Å | 1.76507(192) | 1.76327(178) | 1.75318(277) | 1.75550(231) |
| Mn moment / $\mu_B$ | 2.55(2) | 2.52(2) | 2.56(3) | 2.49(3) |

Previous studies on the structurally related iron arsenide superconductors highlighted that an increasing $T_C$ was correlated to increasingly regular $FeAs_4$ tetrahedra [1–5]. As the F content increases in the Mn samples, the Ce–O/F–Ce bond angles progressively become closer to those of an ideal tetrahedron; the As–Mn–As bond angles do not show a regular trend, but this is presumably due to the As non-stoichiometry in each sample (Table 1, Figure 2).

## Figures

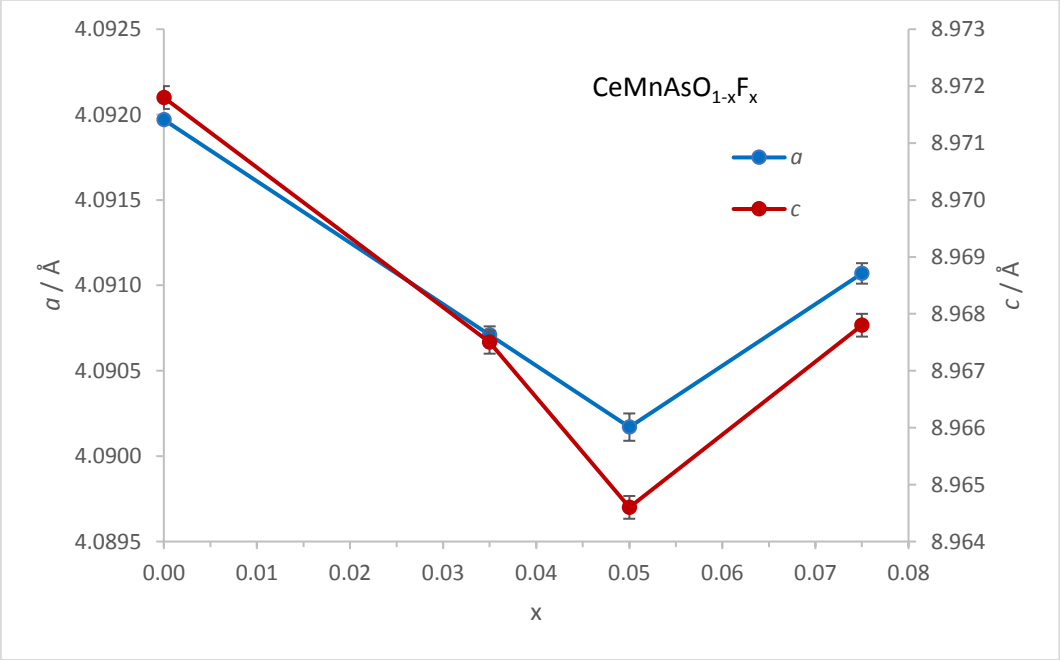


**Figure 1**: Variation of cell parameters for $CeMnAsO_{1-x}F_x$ (x = 0.0, 3.5, 5.0, and 7.5)

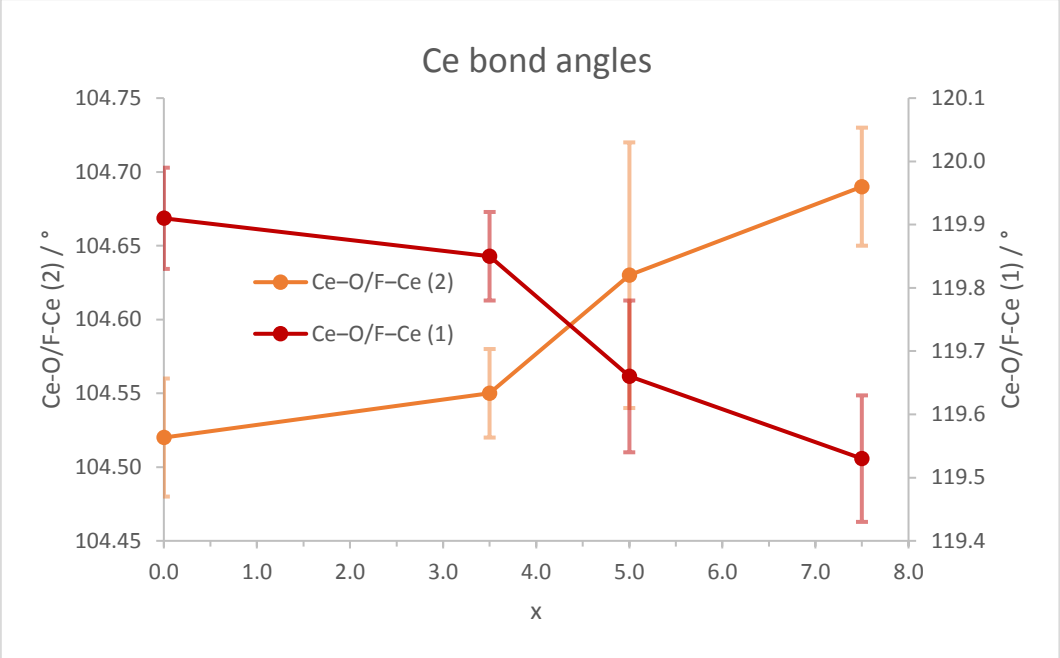


**Figure 2:** Variation in Ce–O/F–Ce bond angles

## References


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