

**Supporting Online Material for:**

**Local structure analysis around Nd center in *ternary* catalyst comprising Nd(vers)<sub>3</sub>, Al(*i*Bu)<sub>3</sub> and Al(*i*Bu)<sub>2</sub>Cl by XAFS**

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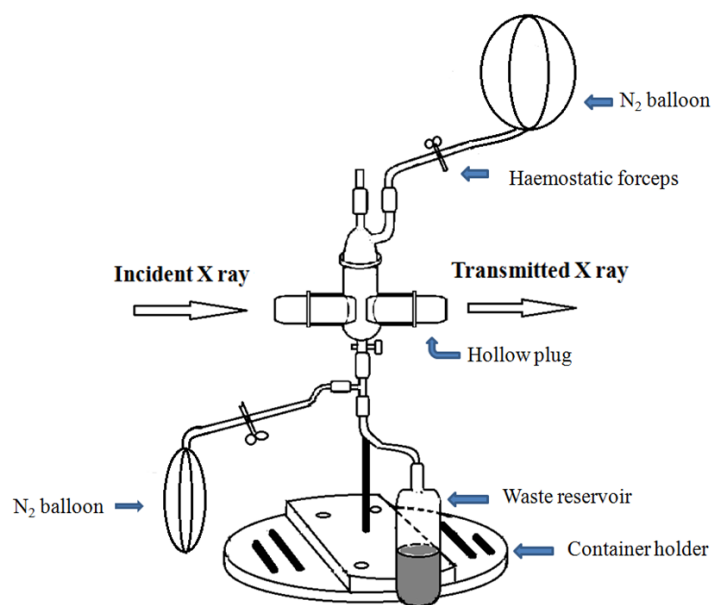
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**Sample-cell design:**

In order to collect the XAFS spectra, a specific sample-cell was designed and manufactured. This sample-cell can protect the sample against moisture and air during the measurements. A sketch map of the homemade sample-cell is shown in [Fig. S1](#). This sample-cell consists of two parts, i.e., a glass liquid container and a metal holder. The liquid container is connected with two N<sub>2</sub> balloons, respectively, at its top and bottom, which can be used to expel the moisture and air from the container and keep the sample out of atmosphere. Meanwhile the N<sub>2</sub> balloons can be also used to compensate the inflation pressure caused by the heat release during the reaction. A waste reservoir is also connected to the liquid container at its bottom, which is used to collect the spent solutions via an outlet. The reagents can be injected into the container through a jam-packed rubber-stopper at its right top. Two hollow plugs with

tetrafluoroethylene film as X-ray windows are face-to-face connected to the container at its waist, which ensure the pass of the X-ray beam. In order to control the thickness of the liquid sample to obtain the optimal XAFS spectra, four rubber rings are tightly covered on each plugs. On the one hand, the thickness of liquid sample can be easily regulated by moving the plugs. On the other hand, the liquid sample can be sealed in the container by the rubber rings. During the XAFS measurements, the container holder was compactly fixed on an experiment platform. The experiment platform can be used to control the tilt, rotation, move-up, and move-down of the container, which guarantee that the X-ray beam pass right through the X-ray windows of the container. After fixing the container holder, the liquid container can be expediently disassembled, cleaned, and reassembled without position change.



**Figure S1.** Schematic diagram of the liquid sample-cell.