Adsorption of fluorinated anesthetics within the pores of a molecular crystal

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Supporting Information

Materials

Enflurane, isoflurane, sevoflurane, methoxyflurane, and halothane were obtained from SynQuest Labs and used without further purification. Ultrahigh purity nitrogen (99.999%) was purchased from Matheson Tri-Gas.

Thermogravimetric Analysis of Anesthetics' Vapor Adsorption

The setup for studying the adsorption of anesthetic vapors is shown in Figure S1. Colorless rod crystals of compound **6**[1] were first heated on a thermobalance of the TA Instruments TGA 2050 thermogravimetric analyzer under N_2 flow to 120 °C at 2 °C/min. This temperature was held for 60 min to ensure complete activation of the material. The temperature was reduced to 25 °C at 5 °C/min and held at 25 °C. The N_2 flow was then switched (red line) to a second N_2 gas stream that was saturated with the vapor of adsorbate at 25 °C (saturation was achieved by passing the N_2 gas stream through a bubbler containing the liquid adsorbate). After the weight reached a plateau, the adsorbate vapor/N_2 flow was switched back to pure N_2 flow at the same temperature (25 °C).

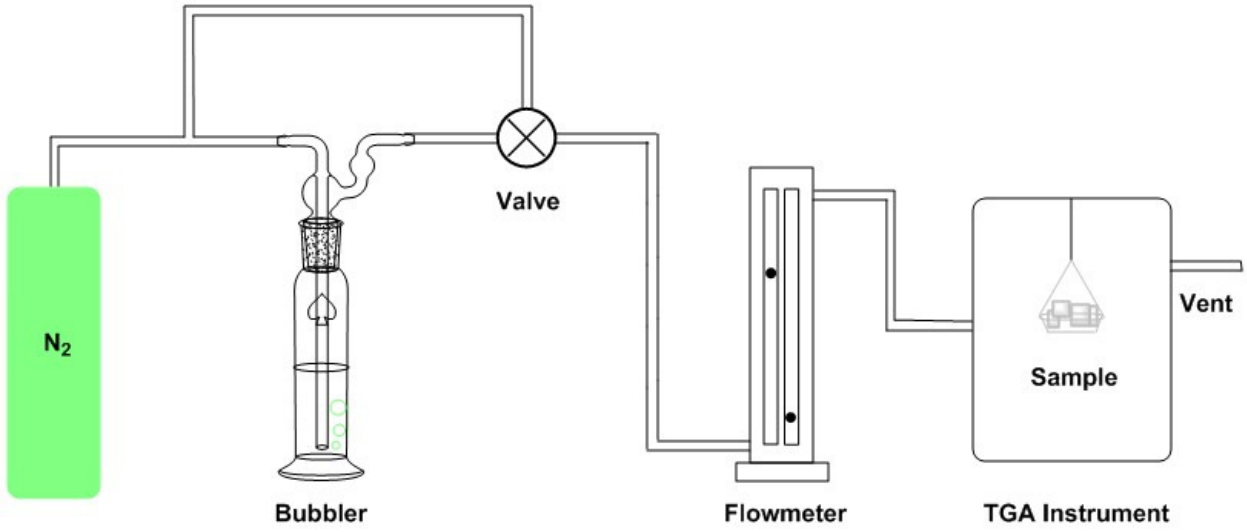

Figure S1. A schematic diagram of the aparatus for TGA of anesthetic vapor adsorption.

Adsorption Results

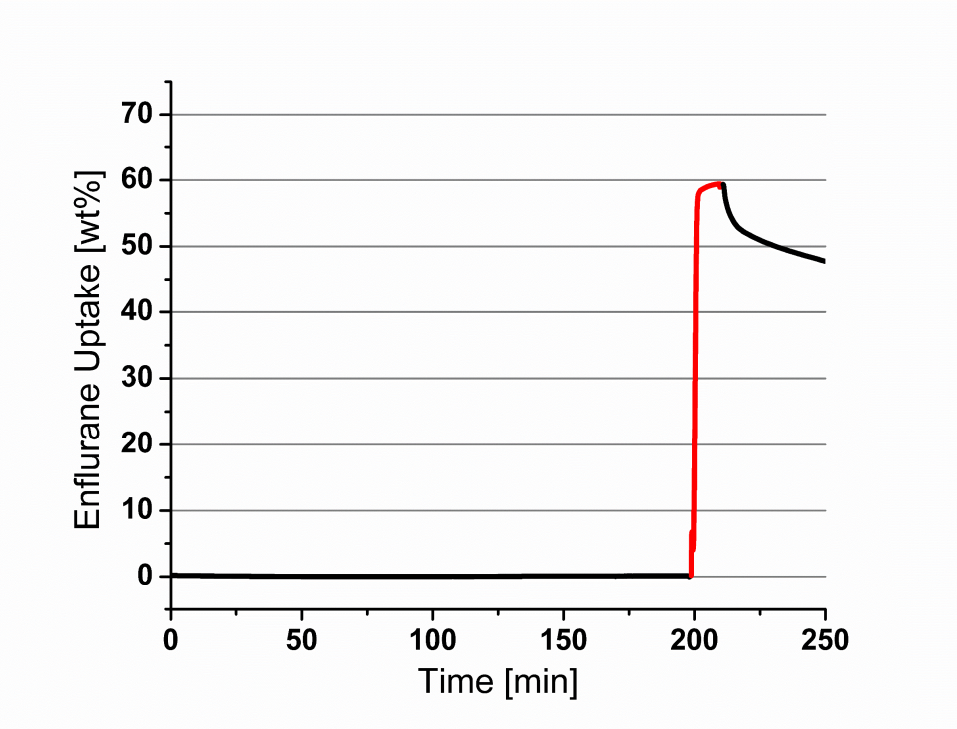

Figure S2. TGA trace for adsorption of enflurane (**1**) within the pores of **6**. Red trace shows the flow of anesthetic-enriched nitrogen, black trace the flow of pure nitrogen.

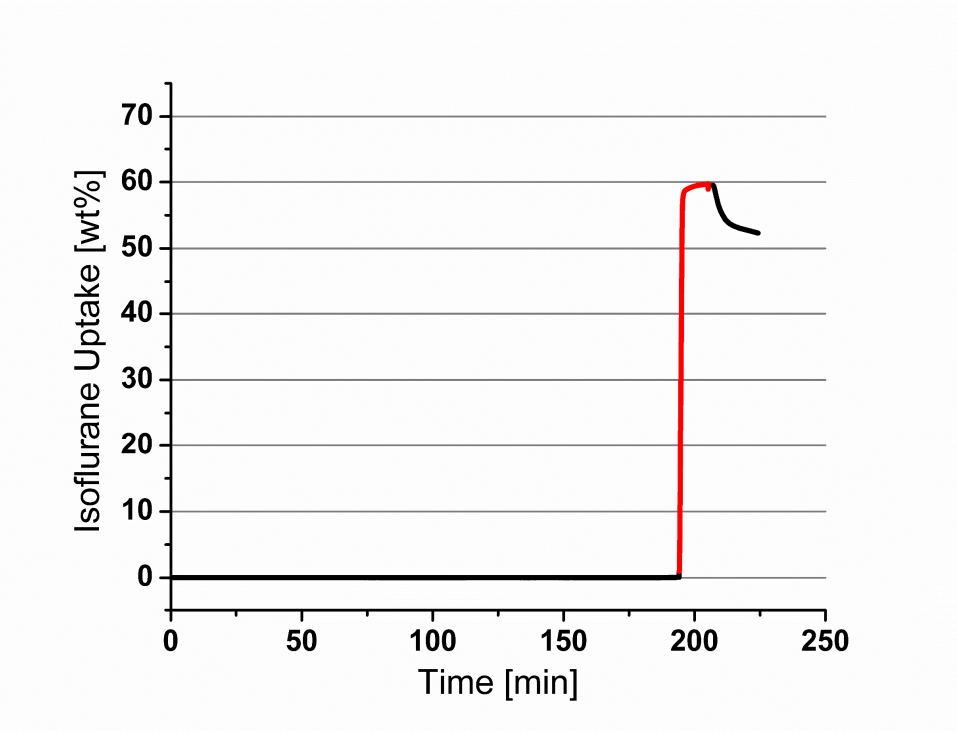

Figure S3. TGA trace for adsorption of isoflurane (**2**) within the pores of **6**. Red trace shows the flow of anesthetic-enriched nitrogen, black trace the flow of pure nitrogen.

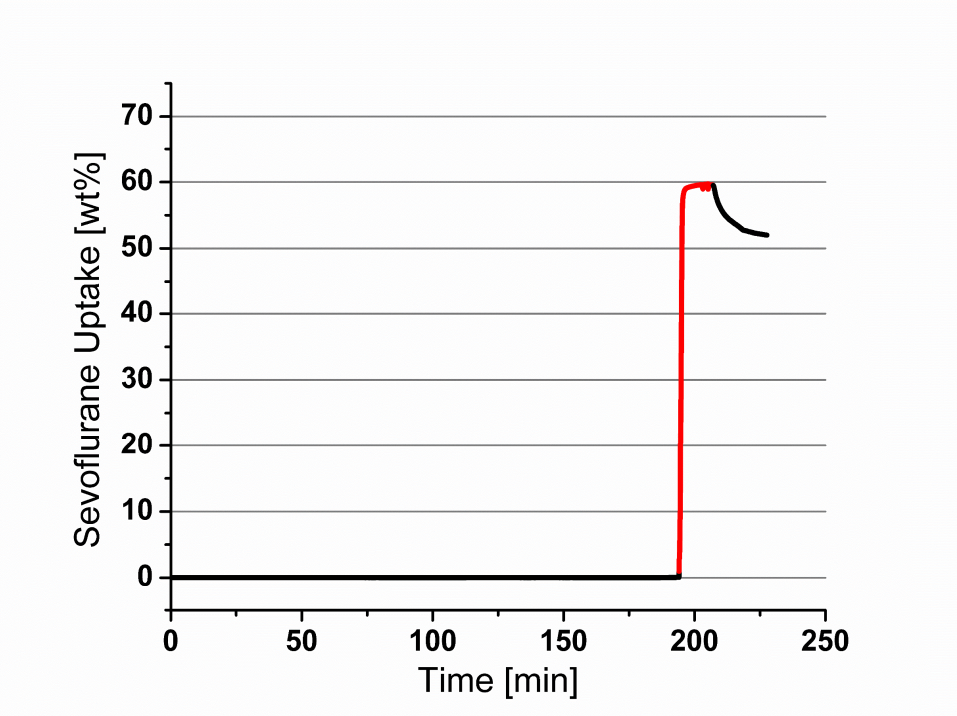

Figure S4. TGA trace for adsorption of sevoflurane (**3**) within the pores of **6**. Red trace shows the flow of anesthetic-enriched nitrogen, black trace the flow of pure nitrogen.

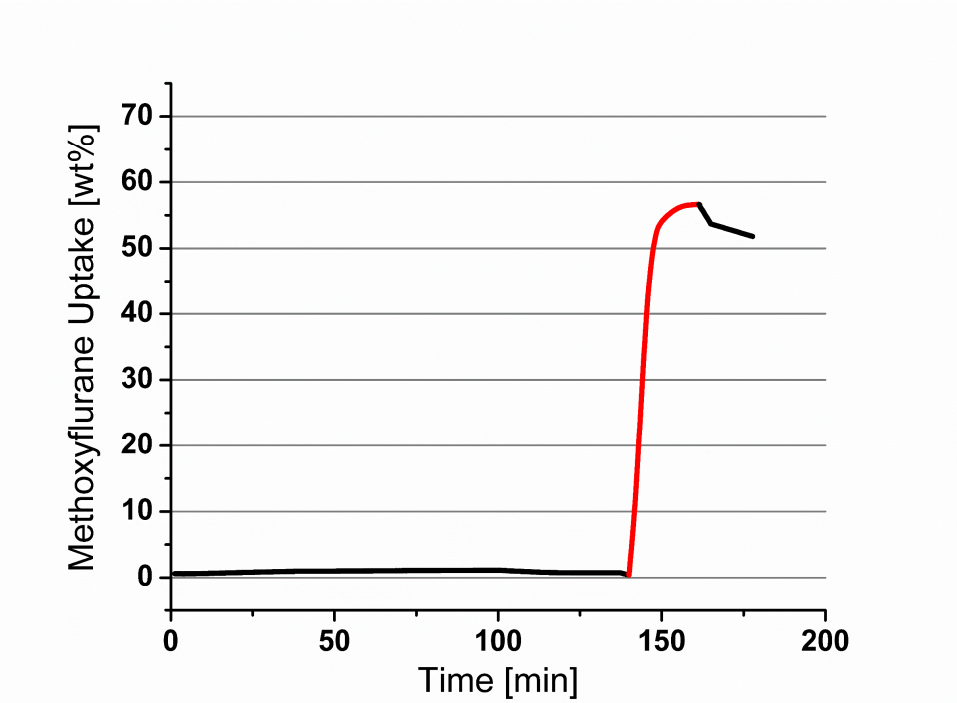

Figure S5. TGA trace for adsorption of methoxyflurane (**4**) within the pores of **6**. Red trace shows the flow of anesthetic-enriched nitrogen, black trace the flow of pure nitrogen.

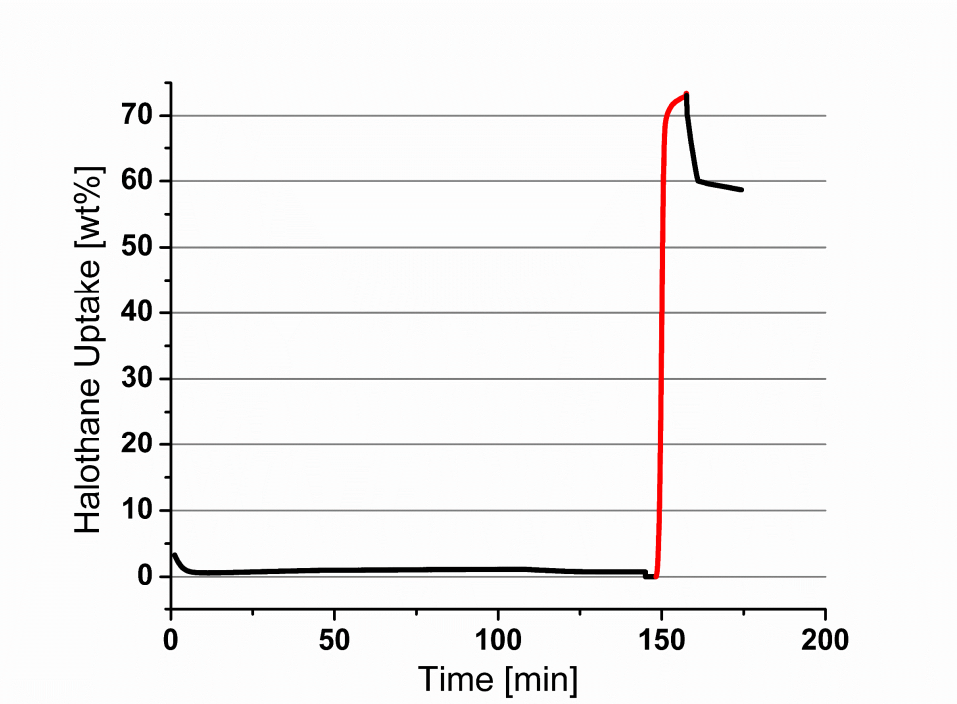

Figure S6. TGA trace for adsorption of halothane (**5**) within the pores of **6**. Red trace shows the flow of anesthetic-enriched nitrogen, black trace the flow of pure nitrogen.

Reference

[1] T.-H. Chen, I. Popov, W. Kaveevivitchai, Y.-C. Chuang, Y.-S. Chen, O. Daugulis, A. J. Jacobson and O. Š. Miljanić, *Nature Commun.*, 2014, **5**, doi: 10.1038/ncomms6131.