Supporting Information

# Highly efficient nitrate ester explosives vapor probe based on multiple triphenylaminopyrenyl-substituted POSS

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## Section 1 TGA Profile

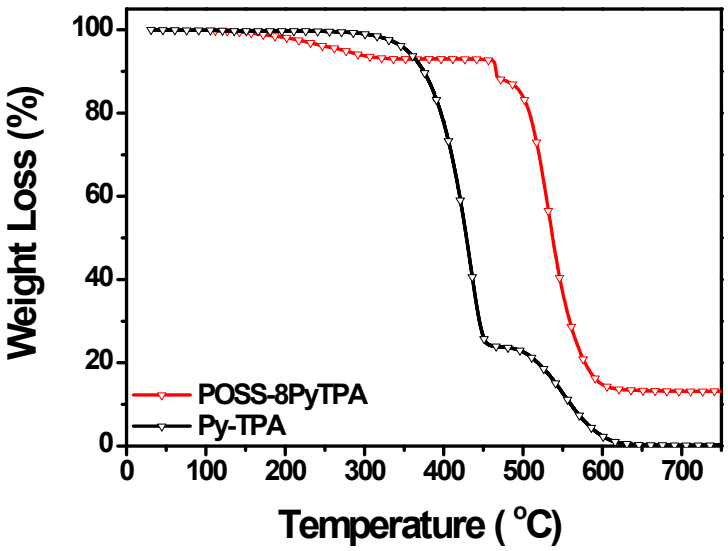



**Fig.S1** TGA curve of **POSS-8PyTPA** and **Py-TPA** under oxygen.

## Section 2 MALDI-TOF Profile

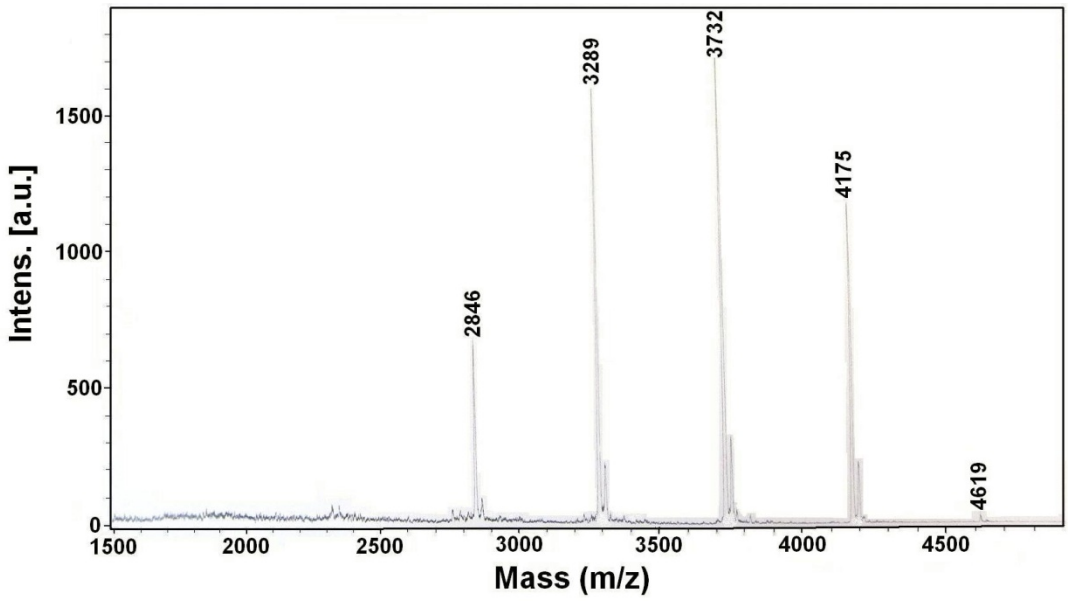
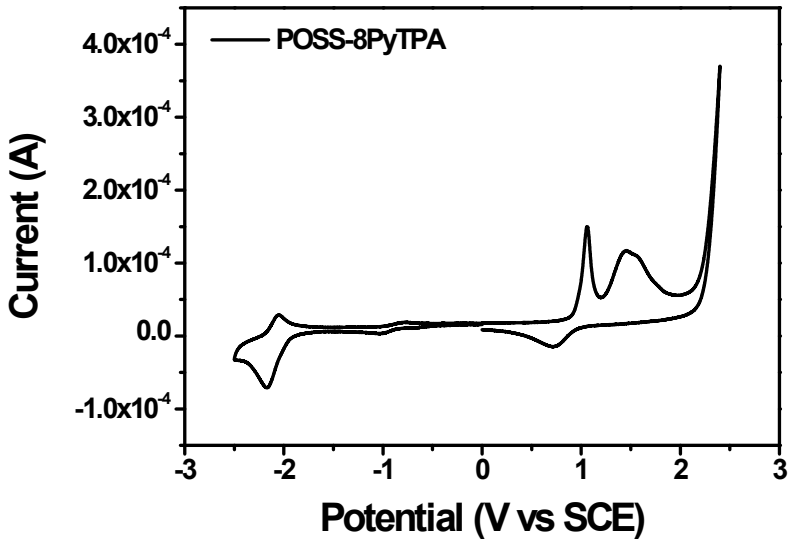



**Fig.S2** MALDI-TOF spectra of **POSS-8PyTPA**.

## Section 3 CV Profile



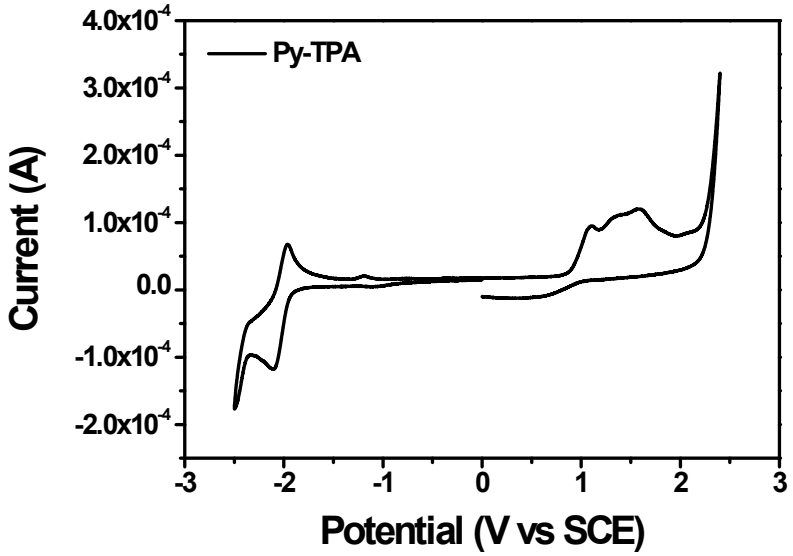
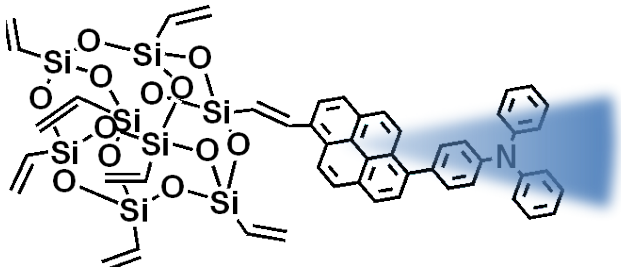



**Fig.S3** Cyclic voltammetric curves of **POSS-8PyTPA** and **Py-TPA**.

## Section 4 Structural Models Calculation Methods

Energy minimization of POSS-8PyTPA was conducted using the Materials Studio version 7.0 program, by means of Geometry Optimization and Dynamics tasks in the Forcite module (Accelrys Software, Inc.). The calculation used a COMPASS II forcefield with atom-based summation for both the electrostatic and van der Waals parameters. Dynamics used a Canonical Ensemble (NVT) ensemble at 298K with Nose method.

## Section 5 Supposition of the Configuration



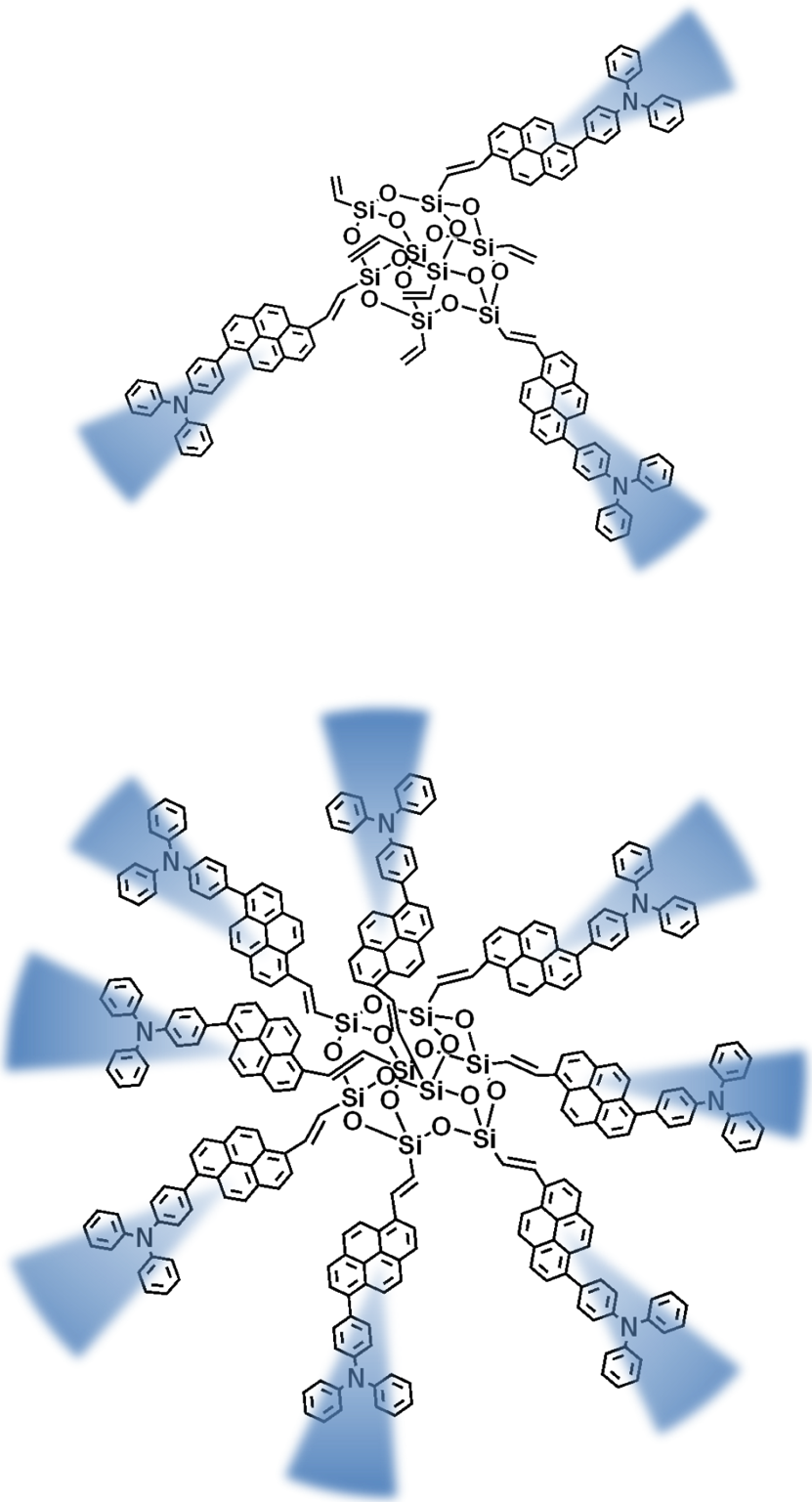


**Fig.S5** The configuration of **P1PT**, **P3PT** and **P8PT**

We suppose the molecular structure of **P1PT**, **P3PT** and **P8PT** as shown in Fig.S5. The

majority of intermolecular interaction comes from Py-TPA units on POSS, while different number of Py-TPA units on POSS (P1PT, P3PT and P8PT) may result in different aggregation behavior. P1PT and P3PT is rather asymmetry in molecular structure, while P8PT are symmetry, therefore P8PT tend to form more smooth aggregation film while P1PT and P3PT prefer random aggregation.