Electronic Supplementary Material (ESI) for RSC Advances.

Support information

Studies on the thermal behavior and safety of the novel thermostable explosive BPTAP

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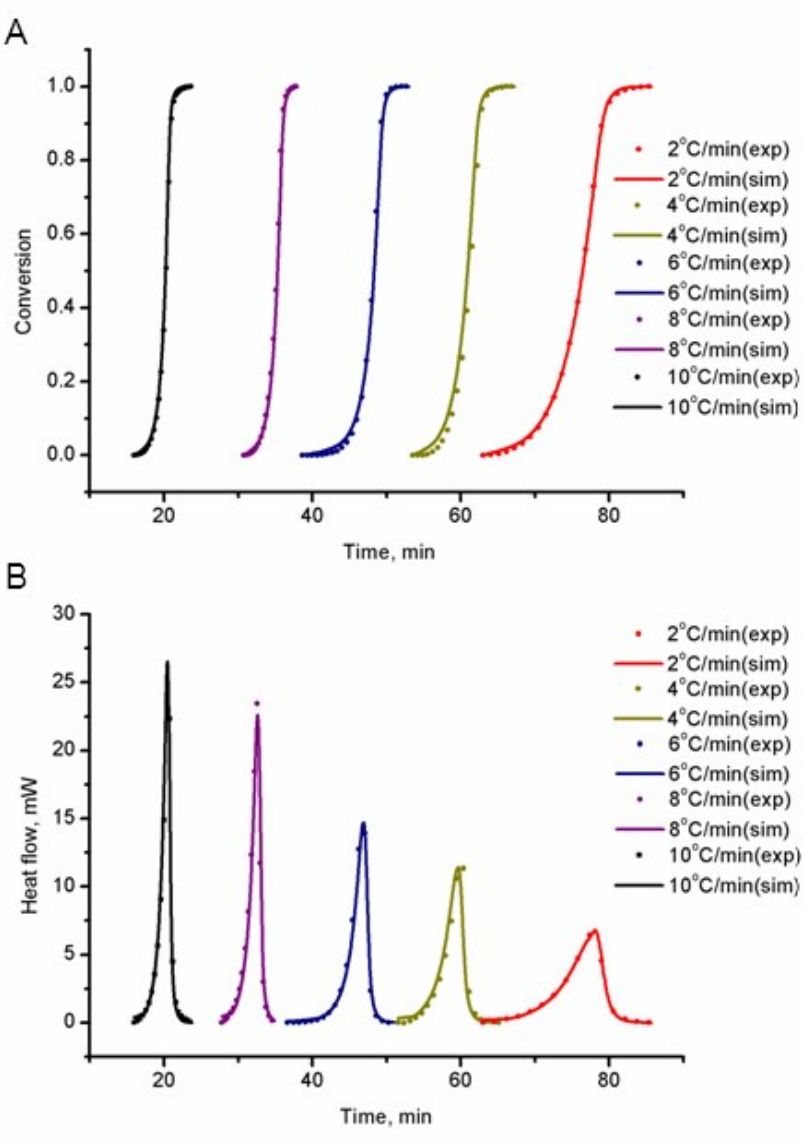

Fig. S1. Experimental and simulated conversion and heat production rate from the DSC data under the hermetic condition. (A) conversion vs time for BPTAP under different temperature rate; (B) heat production rate vs time for BPTAP under different temperature rate.

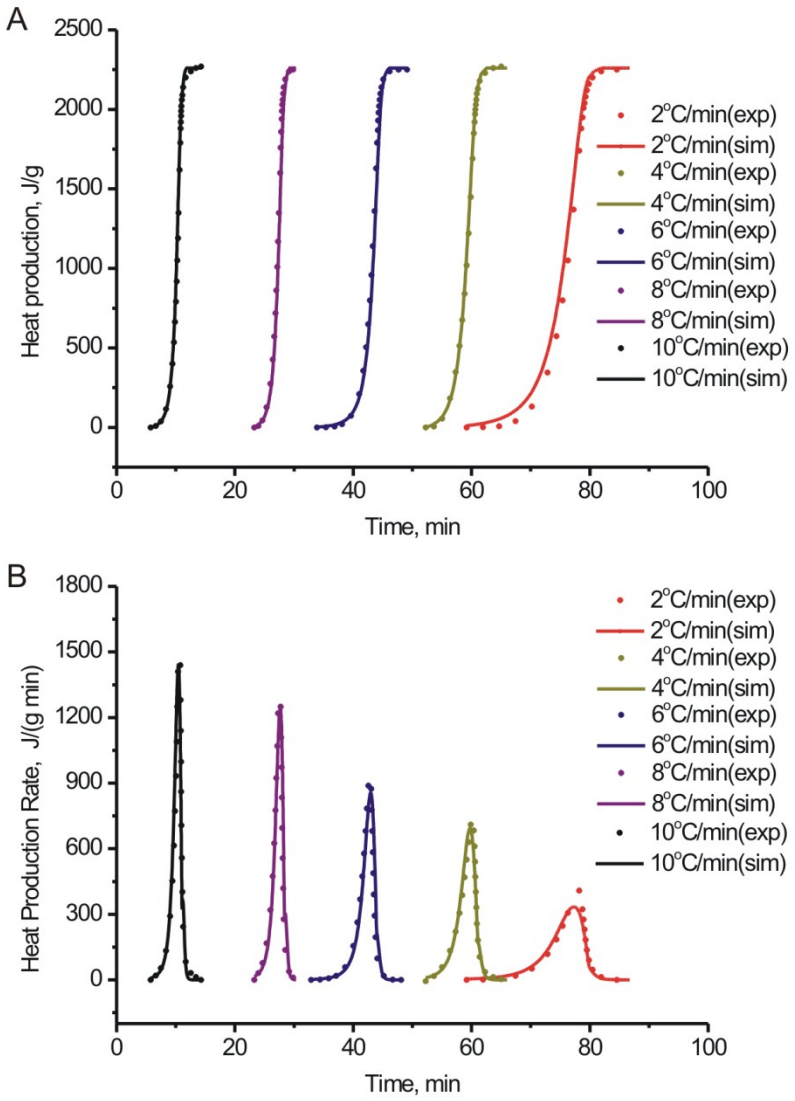

Fig. S2. Comparison between experiment tests in the non-hermetic vessel and simulation of: (A) heat production vs time for BPTAP; (B) heat production rate vs time for BPTAP.

Table S1. Kinetic parameters of the reaction model for BPTAP based on the kinetic model determined in the measurements taken in the hermetic vessel

Parameters	Units	Autocatalytic 1	Autocatalytic 2
ln(A)	$ln(s^{-1})$	25.83	27.97
Ea	kJ mol^{-1}	154.55	172.31
n_1	-	1.18	0.55
n_2	-	1.57	0.87
$ln(z_0)$	-	-5.07	-3.75
Ez	kJ mol^{-1}	1.85	0.05
m	-	0.05	0.05
Q	kJ kg^{-1}	309.78	1952.41