

Supporting Information

The effect of the ball to reactant ratio on mechanochemical reaction times studied by in situ PXRD

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Table 1. Weighed portions and the corresponding BRRs for the reaction of theophylline (TP) and benzoic acid (BA) in molar ratio of 1:1 without SiO₂.

total mass [mg]	mass of TP[mg]	mass of BA [mg]	ball to reactant ratio (BRR)
400	238	162	20
500	298	202	16
600	358	242	13.3
700	417	283	11.4
800	477	323	10
1000	596	404	8

Table 2. Weighed portions and the corresponding BRRs for the reaction of theophylline (TP) and benzoic acid (BA) in molar ratio of 1:1 in the presence of SiO₂.

total mass [mg]	mass of TP[mg]	mass of BA [mg]	mass of SiO ₂ [mg]	ball to reactant ratio (BRR)
1000	238	162	600	20
1000	298	202	500	16
1000	358	242	400	13.3
1000	417	283	300	11.4
1000	477	323	200	10
1000	596	404	0	8

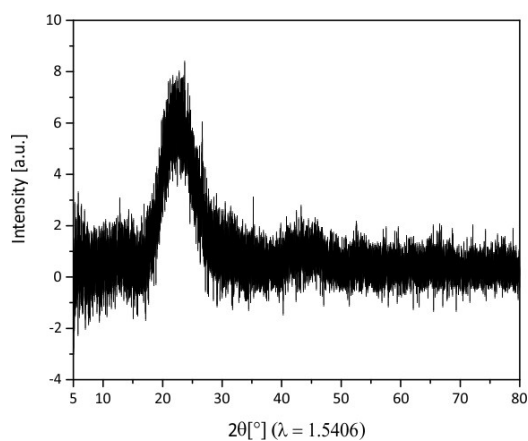


Figure S1. X-ray diffraction pattern of SiO₂ hollow glass spheres.

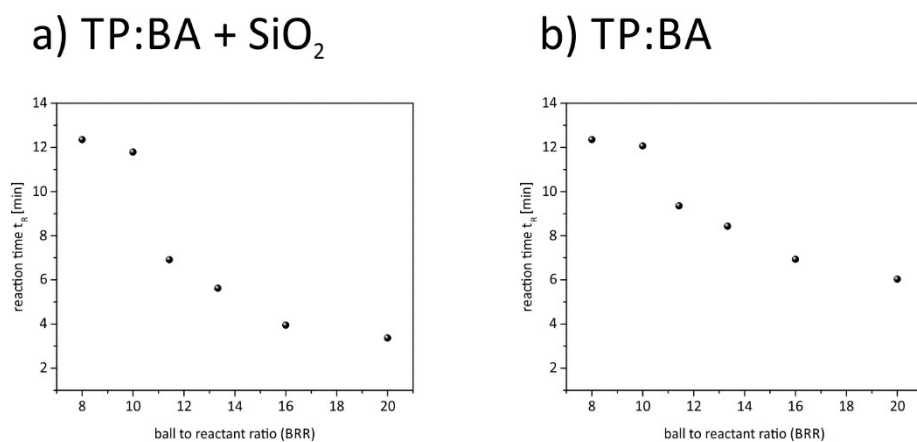


Figure S2. Results of the second run. Reaction times for the cocrystal formation of TP:BA (1:1) as a function of the ball to reactant ratio (BRR) under neat grinding conditions. a) TP and BA (1:1) with weight percentages of 40-100 wt% in the presence of SiO₂ to keep the total load at 1g and b) TP and BA (1:1) with total masses of 400-1000 mg without SiO₂.

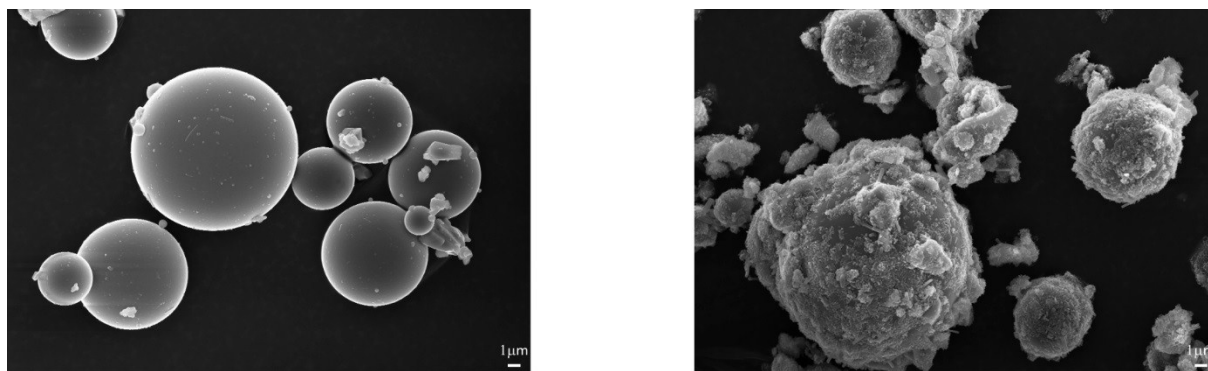


Figure S3. SEM images of SiO_2 hollow spheres before (left) and after (right) grinding for 20 min with theophylline and benzoic acid in molar ratio of 1:1 (40 wt%) to form the TP:BA cocrystal.

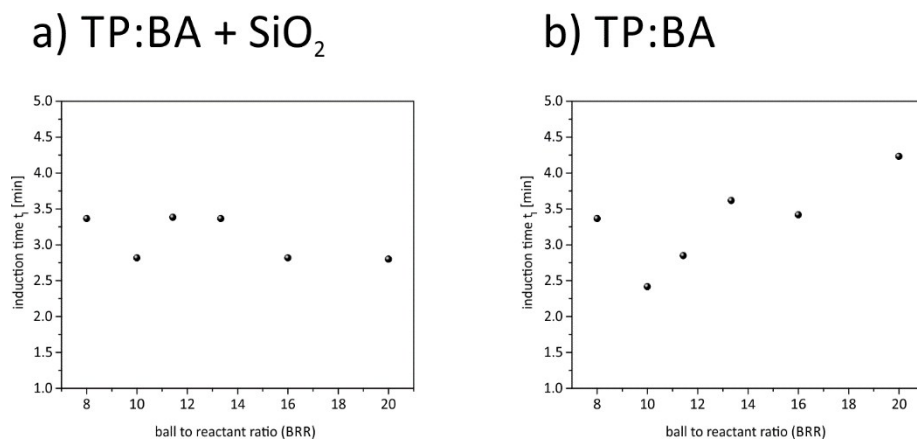


Figure S4. Results of the second run. Induction times for the cocrystal formation of TP:BA (1:1) as a function of the ball to reactant ratio (BRR) under neat grinding conditions. a) TP and BA (1:1) with weight percentages of 40-100 wt% in the presence of SiO_2 and b) TP and BA (1:1) with total masses of 400-1000 mg without SiO_2 .