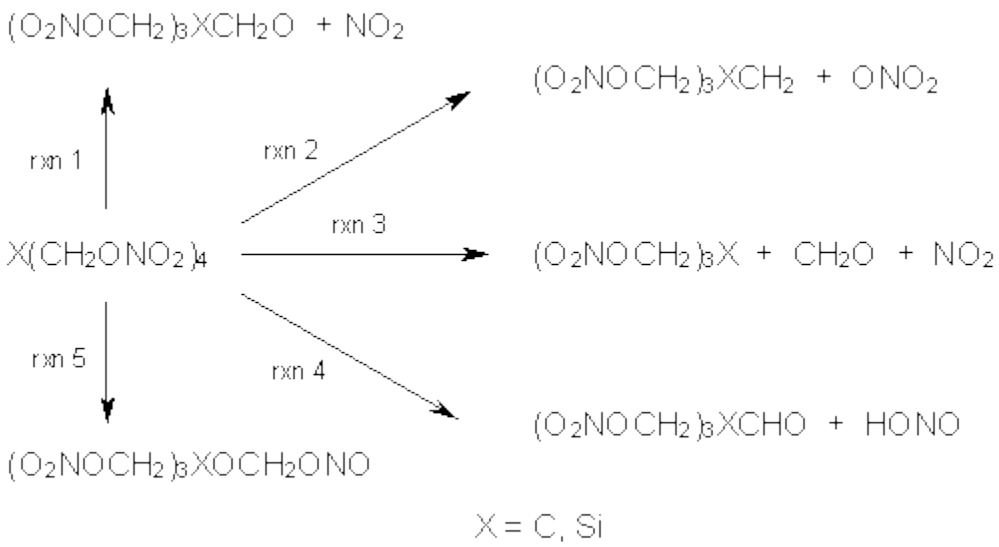
SI-PETN SENSITIVITY EXPLAINED

PETN $C(CH_2ONO_2)_3$ is a relatively insensitive explosive. The silicon analogue $Si(CH_2ONO_2)_3$ is extraordinarily sensitive, exploding at the touch of a spatula. (By the way, this makes it extremely ill-advised as an explosive – it's way too dangerous!) Goddard employed MO6 computations to explore five different possible decomposition pathways, shown in Scheme 1.[1] Reaction 1, the loss of NO_2, is a standard decomposition pathway for many explosives, but the barrier for the C and Si analogues are similar and the reaction of the Si compound is not exothermic. The barrier for Reaction 2 is very large, and the barriers for the C and Si analogues for Reactions 3 and 4 are too similar to explain the differences in their sensitivities.

Scheme 1.



Reaction 5, however, does offer an explanation. The barrier for the Si analogue is 32 kcal mol^{-1}, lower than for any other pathway, and almost 50 kcal mol^{-1} lower than the barrier for the rearrangement of the PETN itself. Furthermore, Reaction 5 is very exothermic for Si-PETN (-44.5 kcal mol^{-1}), while the most favorable pathway for PETN decomposition, Reaction 1, is endothermic. Thus the small barrier and the large amount of energy released for Reaction 5 of Si-PETN suggests its extreme sensitivity.

Source: http://comporgchem.com/blog/?p=258