C. DARKIN

Teetering on the edge

Why do chemists make compounds that could blow up in their faces? Emma Marris finds out… from a safe distance.

Explosives come in many varieties, from military munitions to rapidly inflating airbags. But useful explosives share one thing: stability. A clear advantage of trinitrotoluene, or TNT — whose punch is used as a yardstick for all other explosives — is that it remains safe and solid until detonated. So why would anyone want to make a highly unstable explosive? One that will release its energy on the slightest provocation?

Because they are chemists, and they like explosions, is the popular answer. Because they are chemists, and they like a technical challenge, is what those doing the work say. How convincing is that?

Explosives release energy stored in chemical bonds in a runaway process that often turns solids into gases, expands material massively and creates heat. In big explosions, pressure waves radiate out from the origin, keeping the reaction going throughout the material. When detonated, TNT decomposes violently into a gas, some soot, and a boom. Many explosive compounds are less stable than TNT — some are so temperamental or hard to make that they will probably never be used in practice.

Consider this warning for tetraazidomethane, a particularly wild member of the group of compounds known as polyazides, which have a general reputation for removing student eyebrows. "Tetraazidomethane is extremely dangerous as a pure substance. It can explode at any time — without a recognizable cause."

> "These molecules do not want to exist."
> — Derek Lowe

Klaus Banert at the Chemnitz University of Technology in Germany was the first to synthesize this compound. He says that less than a drop of it destroyed the glass trap and the Dewar flask of the cooling bath they used to isolate it (K. Banert *et al. Angew. Chem. Int. Edn* **46,** 1168–1171; 2007). "Although we had expected explosive properties of tetraazidomethane, we were deeply impressed by its destructive force," he says.

His team had to work behind a safety shield and wear gloves, face shields and ear protectors. Banert says that when it was all over, he was relieved. The lab had taken all reasonable safety precautions but he had still been worried while the experiment was underway.

So why did they do it? Was it the adrenaline? The childhood lure of explosions? Banert says that it was the pure challenge of the synthesis. "I received my first chemistry set at the age of 11 and continued very intensively for several years performing chemical experiments at home. I was also interested in explosives at that time," he says. "But explosions were only of secondary importance."

For tetraazidomethane, Banert says that it was an ambitious target to fill this gap in the family of high-energy density materials. "The structure of tetraazidomethane had already been calculated, and it was predicted that the compound theoretically should be able to exist."

Derek Lowe, a medicinal chemist and author of the popular chemistry blog 'In the Pipeline' runs an occasional item on 'Things I Won't Work With'. Among them are the polyazides. But he can see the appeal of making highly explosive compounds. "These molecules do not want to exist. They are never going to form naturally or spontaneously. These things are teetering right on the edge of not being feasible, and you can be the first to make it."

To strengthen the case that it is the synthesis, not the destruction, that excites such minds, consider the work of Philip Eaton at the University of Chicago, Illinois. In the 1960s, Eaton made cubane — a cube with a carbon at each corner. Then, at the suggestion of an army general, he went on to synthesize a highly explosive compound called octanitrocubane (M.-X. Zhang, P. E. Eaton & R. Gilardi. *Angew. Chem. Int. Edn* **39,** 401–404; 2000). Octanitrocubane has the same pattern, but with nitrogen dioxide bound to each corner carbon atom. "The problem," says Eaton, "was how the devil to make it." The tricky synthesis has, he explains, many, many steps . "In the course of the whole thing we made less than a gram." Eaton can't estimate how much more explosive it is than TNT, except to say "a lot".

The idea was that the density of the structure would pack a high explosive power into a small volume — something that was important to the military when bulky guidance-system computers were hogging too much space in missiles. But octanitrocubane is just too hard to make for it to have any role in the military for the foreseeable future. Eaton is just pleased he figured out how to synthesize it. And he did it, he repeats, for the pure love of the challenge. "The explosiveness has no allure for me at all. I was not the kind of kid who made explosives." The proof? He never set off so much as a milligram of the stuff.

"There may be some folks who like that sort of thing, but they don't tend to last very long," agrees Lowe. "Chemists have a reputation for being closet pyromaniacs, but the real crazies blow themselves up." ■

Emma Marris is a reporter for *Nature* based in Washington DC.