300 years after discovery, structure of mercury fulminate finally determined

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Known to the alchemists and long used as a detonator to set off dynamite—mercury fulminate has a checkered past. Now, more than 300 years after the discovery of this explosive compound, German researchers have been able to characterize its crystal structure and thus finally reveal the molecular structure of mercury fulminate.

As Wolfgang Beck, Thomas Klapötke and their team report in the journal *ZAAC – Journal of Inorganic and General Chemistry*, the orthorhombic crystals consist of separate, nearly linear $Hg(CNO)_2$ molecules.

The alchemists of the seventeenth century were already aware that mixtures of “spiritus vini” (ethanol) and mercury in “aqua fortis” (nitric acid) made for an explosive brew. In his book Laboratorium Chymicum, Johann Kunckel von Löwenstern describes the vigorous reaction of mercury nitrate with alcohol to form mercury fulminate ($Hg(CNO)_2$). In 1799, the English chemist Edward Howard isolated the compound by chance, which was produced a sensation in the nascent scientific field of chemistry.

Mercury fulminate is very sensitive to shock, friction, and sparks. It explosively decomposes to form mercury, carbon monoxide, and nitrogen. This explosive power was used extensively: Alfred Nobel put mercury fulminate into blasting caps for detonating dynamite. This relatively safe new detonator was what allowed for the huge success of dynamite. In Germany alone, the annual production of mercury

fulminate in the early 20th century reached about 100,000 Kg.

The first investigations of the crystal structure of mercury fulminate by X-ray structure analysis date from 1931. Now Beck, Klapötke and their team have finally succeeded in fully solving the structure. To do this, they irradiated small crystals with a uniform crystal lattice, known as single crystals, with X-rays.

The resulting X-ray diffraction pattern allowed the researchers to precisely calculate the positions of the individual atoms within the crystal and the distances between them. Mercury fulminate crystals are orthorhombic and the crystal consists, as expected, of separate $Hg(CNO)_2$ molecules. Each mercury atom is surrounded by two carbon atoms. The measured positions and bond lengths confirm a molecular structure of O–N≡C–Hg–C≡N–O.

Says Beck: “In addition, we can unambiguously show that the molecules in the crystal have a stretched-out, nearly linear form. They are not bent, and each mercury atom is not bound to two oxygen atoms, as they are amazingly still occasionally depicted in the literature.”

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