

Supporting Information

The empirical nitrogen equivalent equation is illustrated as follows:

$$\begin{cases} D = (690 + 1160\rho) \sum N_{\text{ch}} \\ p = 1.106 \left(\rho \sum N_{\text{ch}} \right)^2 - 0.84 \\ \sum N_{\text{ch}} = \frac{100}{M_r} \left(p_i N_{p_i} + \sum B_K N_{B_K} + \sum G_j N_{G_j} \right) \end{cases}$$

D : detonation velocity (m/s)

p : detonation pressure (GPa)

ρ : crystal density of energetic material (g/cm³)

$\sum N_{\text{ch}}$: the total value of nitrogen equivalent coefficient of energetic material

M_r : the molar mass of energetic material

p_i : the total number of i th detonation product with 1 mol explosive exploded completely

N_{p_i} : the total nitrogen equivalent coefficient of i th detonation product

B_K : the total number of K th chemical bond contained in explosive molecule

N_{B_K} : the total nitrogen equivalent coefficient of K th chemical bond

G_j : the total number of j th chemical groups contained in explosive molecule

N_{G_j} : the total nitrogen equivalent coefficient of the j th chemical group.

Nitrogen equivalent coefficient for different detonation products

Detonation product	CO ₂	CO	C	H ₂ O	N ₂
Nitrogen equivalent coefficient	1.279	0.723	0.149	0.626	0.981

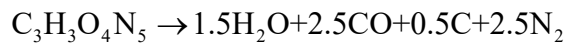
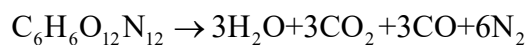
Nitrogen equivalent coefficient for different chemical bonds

Chemical bond	C—C	C—H	C=C	C—N
Nitrogen equivalent coefficient	0.0628	-0.0124	0.0345	0.0090
Chemical bond	N—N	N—H	N≡O	C=N
Nitrogen equivalent coefficient	0.0321	-0.0578	-0.0023	-0.0077

Nitrogen equivalent coefficient for different chemical groups

Chemical group	C—NO ₂	N—NO ₂
Nitrogen equivalent coefficient	0.0016	-0.0028

The detonation equation of CL-20 ($\text{C}_6\text{H}_6\text{O}_{12}\text{N}_{12}$) and LLM-116 ($\text{C}_3\text{H}_3\text{O}_4\text{N}_5$) was illustrated as follows:



The molar mass of CL-20 ($\text{C}_6\text{H}_6\text{O}_{12}\text{N}_{12}$) and LLM-116 ($\text{C}_3\text{H}_3\text{O}_4\text{N}_5$) was illustrated as that:

$$M_r(\text{CL-20}) = 6 \times 12 + 6 \times 1 + 12 \times 16 + 12 \times 14 = 438$$

$$M_r(\text{LLM-116}) = 3 \times 12 + 3 \times 1 + 4 \times 16 + 5 \times 14 = 173$$