Supporting Information

The empirical nitrogen equivalent equation is illustrated as follows:

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

D: detonation velocity (m/s)

p: detonation pressure (GPa)

ρ: crystal density of energetic material (g/cm^3)

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

M_r: the molar mass of energetic material

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

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

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

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

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

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

Nitrogen equivalent coefficient for different detonation products

Detonation product	CO_2	CO	C	H_2O	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 ($C_6H_6O_{12}N_{12}$) and LLM-116 ($C_3H_3O_4N_5$) was illustrated as follows:

$$C_6H_6O_{12}N_{12} \rightarrow 3H_2O+3CO_2+3CO+6N_2$$

$$C_3H_3O_4N_5 \rightarrow 1.5H_2O+2.5CO+0.5C+2.5N_2$$

The molar mass of CL-20 ($C_6H_6O_{12}N_{12}$) and LLM-116 ($C_3H_3O_4N_5$) was illustrated as that:

$$M_r\left(\text{CL-20}\right)=6\times12+6\times1+12\times16+12\times14=438$$

$$M_r\left(\text{LLM-116}\right)=3\times12+3\times1+4\times16+5\times14=173$$